

Table 1	
Variable	Value
1. Age	25.0
2. Sex	Male
3. Education	High school
4. Income	\$10,000
5. Unemployment	10.0
6. Unemployment	10.0
7. Unemployment	10.0
8. Unemployment	10.0
9. Unemployment	10.0
10. Unemployment	10.0
11. Unemployment	10.0
12. Unemployment	10.0
13. Unemployment	10.0
14. Unemployment	10.0
15. Unemployment	10.0
16. Unemployment	10.0
17. Unemployment	10.0
18. Unemployment	10.0
19. Unemployment	10.0
20. Unemployment	10.0
21. Unemployment	10.0
22. Unemployment	10.0
23. Unemployment	10.0
24. Unemployment	10.0
25. Unemployment	10.0
26. Unemployment	10.0
27. Unemployment	10.0
28. Unemployment	10.0
29. Unemployment	10.0
30. Unemployment	10.0
31. Unemployment	10.0
32. Unemployment	10.0
33. Unemployment	10.0
34. Unemployment	10.0
35. Unemployment	10.0
36. Unemployment	10.0
37. Unemployment	10.0
38. Unemployment	10.0
39. Unemployment	10.0
40. Unemployment	10.0
41. Unemployment	10.0
42. Unemployment	10.0
43. Unemployment	10.0
44. Unemployment	10.0
45. Unemployment	10.0
46. Unemployment	10.0
47. Unemployment	10.0
48. Unemployment	10.0
49. Unemployment	10.0
50. Unemployment	10.0
51. Unemployment	10.0
52. Unemployment	10.0
53. Unemployment	10.0
54. Unemployment	10.0
55. Unemployment	10.0
56. Unemployment	10.0
57. Unemployment	10.0
58. Unemployment	10.0
59. Unemployment	10.0
60. Unemployment	10.0
61. Unemployment	10.0
62. Unemployment	10.0
63. Unemployment	10.0
64. Unemployment	10.0
65. Unemployment	10.0
66. Unemployment	10.0
67. Unemployment	10.0
68. Unemployment	10.0
69. Unemployment	10.0
70. Unemployment	10.0
71. Unemployment	10.0
72. Unemployment	10.0
73. Unemployment	10.0
74. Unemployment	10.0
75. Unemployment	10.0
76. Unemployment	10.0
77. Unemployment	10.0
78. Unemployment	10.0
79. Unemployment	10.0
80. Unemployment	10.0
81. Unemployment	10.0
82. Unemployment	10.0
83. Unemployment	10.0
84. Unemployment	10.0
85. Unemployment	10.0
86. Unemployment	10.0
87. Unemployment	10.0
88. Unemployment	10.0
89. Unemployment	10.0
90. Unemployment	10.0
91. Unemployment	10.0
92. Unemployment	10.0
93. Unemployment	10.0
94. Unemployment	10.0
95. Unemployment	10.0
96. Unemployment	10.0
97. Unemployment	10.0
98. Unemployment	10.0
99. Unemployment	10.0
100. Unemployment	10.0

Serial No.: To Be Assigned

Title: DERIVING CHEMICAL STRUCTURAL INFORMATION

COVER SHEET FOR APPENDIX: NOMTOKENS

Enclosed for filing in the above-referenced patent application is the following document:

1. Appendix: NOMTOKENS, 111 pages.

Respectfully submitted,

Jason A. Reyes
Registration No. 41,513
Attorney for Applicant

Attorney Docket No. 103544.127

EXPRESS MAIL LABEL NO. EM259723548US
DATE OF DEPOSIT February 11, 2000

meth|carbin root alkane C,a|alpha|1|w|omega
 carbenium root root [C+],1|w|omega
 carbene root root C,32@1|w|omega
 aminylene|nitrene root root N,32@1|w|omega
 hydroxymethyl root root C,4@x,0,x
 hydroxymethylene root root C,8@x,0,x
 form root trivial C,x|1|w|omega,(=O),x
 formimino root trivial C,4@x|1|w|omega,(=N),x
 formalin root root C=O,x
 eth root alkane C,1|a|alpha,C,2|b|beta|w|omega
 ethene|ethen root alkane C,1|a|alpha,=,x,C,2|b|beta|w|omega
 ethyne|ethyn root alkane C,1|a|alpha,#,x,C,2|b|beta|w|omega
 acet root trivial C,1,(=,x,0,x),x,C,2|a|alpha|w|omega
 aceto root trivial C,4@1,(=,x,0,x),x,C,2|a|alpha|w|omega
 acetoacet|acetoaceto root trivial
 C,1,(=,x,0,x),x,C,2|a|alpha,C,3,(=,x,0,x),x,C,4|g|gamma|w|omega
 prop|propa root alkane C,1|a|alpha,C,2|b|beta,C,3|g|gamma|w|omega
 isoprop|isopropa|isopropion root alkane C,a|alpha,(x,C,b|beta),x,C,x
 hexafluoroisoprop|hexafluoroisopropa root alkane
 C,a|alpha,(C(F)(F)F),x,C(F)(F)F,x
 propiono|propion|propio|propi root trivial
 C,1,(=,x,0,x),x,C,2|a|alpha,C,3|b|beta|w|omega
 proparg|proparag root alkane C,1|a|alpha,C,2,#,x,C,3|w|omega
 tetrol|loveracid alkane C,1,C,2,#,x,C,3,C,4|w|omega
 but|buta root alkane C,1|a|alpha,C,2|b|beta,C,3|g|gamma,C,4|d|delta|w|omega
 butyro|butyr root trivial
 C,1,(=,x,0,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma|w|omega
 isobutyro|isobutyr root trivial
 C,1,(=,x,0,x),x,C,2|a|alpha,(x,C,3|b|beta),x,C,4|b'|beta'|g|gamma|w|omega
 isobutylene root root C=C(C)C,x
 crotono|croton root trivial
 C,1,(=,x,0,x),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
 crot root root C,1,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
 crotonylalcohol root root
 C,1,(O),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
 isocrotono|isocroton root trivial
 C,1,(=,x,0,x),x,/,x,C,2|a|alpha,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega
 isocrot root root C,1,/,x,C,2|a|alpha,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega
 seneci root trivial
 C,1,(=,x,0,x),x,C,2|a|alpha,=,x,C,3|b|beta,(x,C,4|g|gamma|w|omega),x,C,4'|g'|gamma'|w'|omega
 tig1|cevad root trivial
 C,1,(=,x,0,x),x,/,x,C,2|a|alpha,(C),x,=,x,C,3|b|beta,/,x,C,4|g|gamma|w|omega
 angel root trivial
 C,1,(=,x,0,x),x,/,x,C,2|a|alpha,(C),x,=,x,C,3|b|beta,\,x,C,4|g|gamma|w|omega
 pren root alkane C,1,C,2|a|alpha,=,x,C,3|b|beta,(C),x,C,4|g|gamma|w|omega
 valero|valer|valerian root trivial
 C,1,(=,x,0,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega
 acetoxal root trivial
 C,1,(=,x,0,x),x,C,2|a|alpha,(=O),x,C,3|b|beta,C,4|g|gamma,(=O),x,C,5|d|delta|w|omega
 valpr root trivial
 C,1,(=,x,0,x),x,C,2|a|alpha,(CCC),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega
 levulin|laevulin|levul root trivial
 C,1,(=,x,0,x),x,C,2|a|alpha,C,3|b|beta,C,4,(=O),x,C,5|g|gamma|d|delta|w|omega
 isovalero|isovaler|delphin root trivial
 C,1,(=,x,0,x),x,C,2|a|alpha,C,3|b|beta,(x,C,4|g|gamma),x,C,5|d|delta|w|omega

pival root trivial
 $C,1,(=,x,O,x),x,C,2|a|alpha,(x,C,3|b|beta),(x,C,4|3',),x,C,5|3''$
 amyl root alkane $C,4@1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta|w|omega$
 capro root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon|w|omega$
 acexam root root
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,N,x,C,x,(=O),x,C,x,$
 enatho|enanth|oenantho|oenanth root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7|w|omega$
 geron root trivial
 $C,1,(=,x,O,x),x,C,2|a|alpha,(C)(C),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,(=O),x,C,7|w|omega$
 capryl root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8|w|omega$
 octoate root root
 $O,1@x,C,1,(=O),x,C,2|a|alpha,(x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,n),x,C,x,C,x$
 pelargono|pelargon|pelarg|pergon root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9|w|omega$
 mega
 capr root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10|w|omega$
 obtusil root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10|w|omega$
 stilling root alkane
 $C,1/,x,C,2|a|alpha,=,x,C,3|b|beta,/,x,C,4|g|gamma,=,x,C,5|d|delta,\backslash,x,C,6|e|epsilon,C,7,C,8,C,9,C,10|w|omega$
 lauro|laur|vulv|laurostear root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12|w|omega$
 linder root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12|w|omega$
 myristo|myrist root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14|w|omega$
 physeter|physoter root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,=,x,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14|w|omega$
 ipurol root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,(O),x,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,(O),x,C,12,C,13,C,14|w|omega$
 tsuzu|tudu root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14|w|omega$
 myristelaid root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,=,x,C,10,/,x,C,11,C,12,C,13,C,14|w|omega$
 myristole root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,=,x,C,10,\backslash,x,C,11,C,12,C,13,C,14|w|omega$
 palmito|palmit|cet root alkane
 $C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16|w|omega$

palmitelaid root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,/,x,C,11,C,12,C,13,C,14,C,15,C,16|w|omega

palmitole root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,\,x,C,11,C,12,C,13,C,14,C,15,C,16|w|omega

hiragon root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,=,x,C,7,C,8,C,9
 ,C,10,=,x,C,11,C,12,C,13,C,14,=,x,C,15,C,16|w|omega

ustil root alkane

C,1,C,2|a|alpha,(0),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C
 ,9,C,10,C,11,C,12,C,13,C,14,C,15,(0),x,C,16|w|omega,0,x

ambrettol root alkane

C,1,C,2|a|alpha,(0),x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,=,x,C
 ,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16|w|omega,0,x

aleurit root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(0)
 ,x,C,10,(0),x,C,11,C,12,C,13,C,14,C,15,C,16|w|omega,0,x

gaid|hypogae root alkane

C,1,C,2|a|alpha,=,x,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9
 ,C,10,C,11,C,12,C,13,C,14,C,15,C,16|w|omega

juniper root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16|w|omega,0,x

margaro|margar root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17|w|omega

stear|stearophan root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

moroct root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,=,x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,=,x
 ,C,9,C,10,C,11,C,12,=,x,C,13,C,14,C,15,=,x,C,16,C,17,C,18|w|omega

parinar root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,=,x
 ,C,10,C,11,=,x,C,12,C,13,=,x,C,14,C,15,=,x,C,16,C,17,C,18|w|omega

eleostear root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,\,x,C,11,=,x,C,12,/,x,C,13,=,x,C,14,\,x,C,15,C,16,C,17,C,18|w|omega

stearol loveracid root

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,#,x
 ,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

couep|lican root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,(=0),x,C,5|d|delta,C,6|e|epsilon,C,7,C,8,
 C,9,=,x,C,10,C,11,=,x,C,12,C,13,=,x,C,14,C,15,C,16,C,17,C,18|w|omega

trichosan root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9
 ,=,x,C,10,/,x,C,11,=,x,C,12,\,x,C,13,=,x,C,14,/,x,C,15,C,16,C,17,C,18|w|omega

floionol|phloionol root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,(0)
 ,x,C,10,(0),x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega,0,x

lycaon root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,1
 0,C,11,C,12,(=0),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

lactarin root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,(=0),x,C,7,C,8,
 C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

jalapinol root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,(O),x,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

ole root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

elaaid root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

ricinole|ricinol root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,[C@H],12,(O),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

ricinelaid root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,[C@H],12,(O),x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

linole|telfair root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,C,15,C,16,C,17,C,18|w|omega

vermol loveracid root CCCCCC\C=C/C[C@H]1[C@H](CCCC)O1,x

linolelaid root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,C,15,C,16,C,17,C,18|w|omega

linolenelaid root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,/,x,C,15,/,x,C,16,/,x,C,17,C,18|w|omega

omega

linolen|alphalinolen root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,/,x,C,15,/,x,C,16,/,x,C,17,C,18|w|omega

omega

gammalinolen root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,/,x,C,7,/,x,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,C,15,C,16,C,17,C,18|w|omega

omega

vaccen root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,/,x,C,11,/,x,C,12,/,x,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

petroselaid root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,/,x,C,7,/,x,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

petroselin root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,/,x,C,6|e|epsilon,/,x,C,7,/,x,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18|w|omega

calend root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,/,x,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,C,15,C,16,C,17,C,18|w|omega

arachido|arachid|arachin root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20|w|omega

gadole root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,/,x,C,9,/,x,C,10,/,x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,18,C,19,C,20|w|omega

arachidon root alkane

C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,/,x,C,5|d|delta,/,x,C,6|e|epsilon,/,x,C,7,/,x,C,8,/,x,C,9,/,x,C,10,/,x,C,11,/,x,C,12,/,x,C,13,/,x,C,14,/,x,C,15,/,x,C,16,C,17,C,18,C,19,C,20|w|omega

lesquerol root alkane

beheno|behen root alkane

eruc root alkane

brassid root alkane

lignocero|lignocer root alkane

cerebron|phrenosin root alkane

nervon root alkane

hyen root alkane

cerotino|cerotin|cerot|cerane root alkane

ceryl root alkane

cluyt	montano	montan	root	alkane
-------	---------	--------	------	--------

melisso|meliss|myric root alkane

laccero|laccer root alkane

acroleine|acrolein root root C,1,(=,x,0,x,),x,C,2|a|alpha,=,x,C,3|b|beta|w|omega

methacrolein root root C,1,(=,x,0,x,) ,x,C,2|a|alpha,(C),x,=,x,C,3|b|beta|w|omega

acr root trivial C,1,(=,x,0,x,),x,C,2|a|alpha,=,x,C,3|b|beta|w|omega

```
hydracr root trivial C,1,(=,x,0,x),x,C,2,C,3|w|omega,0,o
```


adipo|adip root diacid
C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,4@6,=,x,O,x
glutacon|glutacono root diacid C,1,(=,x,O,x),x,C,2,=,x,C,3,C,4,C,4@5,=,x,O,x
mucon|mucono root diacid C,1,(=,x,O,x),x,C,2,=,x,C,3,C,4,=,x,C,5,C,4@6,=,x,O,x
dihydromucon|dihydromucono root diacid
C,1,(=,x,O,x),x,C,2,=,x,C,3,C,4,C,5,C,4@6,=,x,O,x
pimelo|pimel|piler root diacid
C,1,(=,x,O,x),x,C,2,C,3,C,4,C,5,C,6,C,4@7,=,x,O,x
subero|suber root diacid
C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,4@8,=,x,O,x
azela|azele|azel|lepargyl root diacid
C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,4@9,=,x,O,x
sebaco|sebac root diacid
C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,9,C,4@10,=,x,O,x
traumat|traumato root diacid
C,1,(=,x,O,x),x,C,2,=,x,C,3,C,4,C,5,C,6,C,7,C,8,C,9,C,10,C,11,C,4@12,=,x,O,x
brassylo|brassyl root diacid
C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,4@13,=,x,O,x
thapso|thaps root diacid
C,1,(=,x,O,x),x,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15,C,4@16,=,x,O,x
floion|phloion root diacid
C,1,(=,x,O,x),x,C,2,C,3,C,4,C,5,C,6,C,7,C,8,C,9,(O),x,C,10,(O),x,C,11,C,12,C,13,C,14,C,15,C,16,C,17,C,4@18,=,x,O,x
folin root diacid
C,x,(=,x,O,x),x,(C(CC,x,C,4@x,=O)NC(C(C=C3)=CC=C3NCC(CN2)N(C=O)C1=C2N=C(N)NC1=O)=O),x
spiculspor root diacid
C,x,(=,x,O,x),x,Ring,Ring1,.,x,C,1,(x,=,x,O,x),x,(x,O,x,Ring,Ring2),x,C,2,C,3,C,4,Ring,Ring2,Ring,Ring1,C,5,(x,C,4@x,=,x,O,x),x,C,6,C,7,C,8,C,9,C,10,C,11,C,12,C,13,C,14,C,15
chaulmoogr root alkane
C,1,C,2|a|alpha,C,3|b|beta,C,4|g|gamma,C,5|d|delta,C,6|e|epsilon,C,7,C,8,C,9,C,10,C,11,C,12,C,13,[C@@H],x,Ring,Ring1,c,x,c,x,C,x,C,x,Ring,Ring1
pyrocarbon root diacid C,x,(=,x,O,x),x,O,x,C,4@x,=,x,O,x
imidodicarbon|iminodicarbon root diacid C,x,(=,x,O,x),x,N,n,C,4@x,=,x,O,x
pyrocarbon root diacid C,x,(=,x,O,x),x,O,x,C,4@x,=,x,O,x
thiodicarbon root diacid C,x,(=,x,O,x),x,S,x,C,4@x,=,x,O,x
peroxydicarbon root diacid C,x,(=,x,O,x),x,OO,x,C,4@x,=,x,O,x
thioperoxydicarbon root diacid C,x,(=,x,O,x),x,SS,x,C,4@x,=,x,O,x
chelidon|chelid root diacid C,x,(=,x,O,x),x,c1cc(=O)cc(o1),x,C,4@x,=,x,O,x
pamo|embon root diacid
C,x,(=,x,O,x),x,C1=CC3=C(C=CC=C3)C(CC2=C(C=CC=C4)C4=CC(x,C,4@x,=,x,O,x)=C2O)=C1O,x
citr root polyacid C,1,C,2,C,3,(x,O,x),x,(x,C,x),x,C,x,C,x
isocitr root polyacid C,x,C,x,(x,O,x),x,C,x,(x,C,x),x,C,x,C,x
tricarballyl root polyacid C,x,C,x,C,x,(x,C,x),x,C,x,C,x
aconit root polyacid C,x,C,x,=,x,C,x,(x,C,x),x,C,x,C,x
trimellit root polyacid
C,x,c,1,Ring,Ring1,c,2,(x,C,x),x,c,3,c,4,c,5,(x,C,x),x,c,6,Ring,Ring1
hemimellit root polyacid
C,x,c,1,Ring,Ring1,c,2,(x,C,x),x,c,3,(x,C,x),x,c,4,c,5,c,6,Ring,Ring1

hemimellitene root root
C,x,c,1, Ring, Ring1, c, 2, (, x, C, x,), x, c, 3, (, x, C, x,), x, c, 4, c, 5, c, 6, Ring, Ring1
pyromellit root polyacid
C,x,c,1, Ring, Ring1, c, 2, (, x, C, x,), x, c, 3, c, 4, (, x, C, x,), x, c, 5, (, x, C, x,), x, c, 6, Ring, Ring1
pyromellitene root root
C,x,c,1, Ring, Ring1, c, 2, (, x, C, x,), x, c, 3, c, 4, (, x, C, x,), x, c, 5, (, x, C, x,), x, c, 6, Ring, Ring1
mellit root polyacid
C,x,c,1, Ring, Ring1, c, 2, (C), x, c, 3, (C), x, c, 4, (C), x, c, 5, (C), x, c, 6, (C), x, Ring, Ring1
trimes root polyacid
C,x,c,1, Ring, Ring1, c, 2, c, 3, (, x, C, x,), x, c, 4, c, 5, (, x, C, x,), x, c, 6, Ring, Ring1
mellophan root polyacid
C,x,c,1, Ring, Ring1, c, 2, (C), x, c, 3, (C), x, c, 4, (C), x, c, 5, c, 6, Ring, Ring1
prehnit root polyacid
C,x,c,1, Ring, Ring1, c, 2, (C), x, c, 3, (C), x, c, 4, c, 5, (C), x, c, 6, Ring, Ring1
berberon|beron root polyacid
C,x,c,2, Ring, Ring1, c, 3, (, x, C, x,), x, c, 4, c, 5, (, x, C, x,), x, c, 6, n, 1, Ring, Ring1
phthalide root root
O, x, =, x, C, 1, Ring, Ring1, O, 2, C, 3 | a | alpha, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring1, Ring, Ring2
phthalane|phthalan root root
C, 1, Ring, Ring1, O, 2, C, 3, C, 3a, Ring, Ring2, =, x, C, 4, C, 5, =, x, C, 6, C, 7, =, x, C, 7a, Ring, Ring1, Ring, Ring2
phthalo|phthal|orthophthal root diacid
C, x, (=, x, O, x,), x, c, 1, Ring, Ring1, c, 2, (, x, C, 4@x, =, x, O, x,), x, c, 3, c, 4, c, 5, c, 6, Ring, Ring1
homophthalo|homophthal root diacid
C, x, (=, x, O, x,), x, c, 1, Ring, Ring1, c, 2, (, x, C, x, C, 4@x, =, x, O, x,), x, c, 3, c, 4, c, 5, c, 6, Ring, Ring1
isophthalo|mpthalo|isophthal|mpththal root diacid
C, x, (=, x, O, x,), x, c, 1, Ring, Ring1, c, 2, c, 3, (, x, C, 4@x, =, x, O, x,), x, c, 4, c, 5, c, 6, Ring, Ring1
terephthalo|ppthalo|terephthal|ppththal root diacid
C, x, (=, x, O, x,), x, c, 1, Ring, Ring1, c, 2, c, 3, c, 4, (, x, C, 4@x, =, x, O, x,), x, c, 5, c, 6, Ring, Ring1
uvit root diacid
C, x, (=, x, O, x,), x, c, 1, Ring, Ring1, c, 2, c, 3, (, x, C, 4@x, =, x, O, x,), x, c, 4, c, 5, (C), x, c, 6, Ring, Ring1
leucate|leucicacid root root
C, 1, (=, x, O, x,), x, (, x, O, 1@x,), x, C, 2, (, x, O, x,), x, C, 3, C, 4, (, x, C, 5,), x, C, x
phenylephrine|phenylephrin root root Oc1cccc(C(O)CNC)c1, x
norepinephrine|norepinephrin|noradrenaline|noradrenalin|arterenol root root
Oc1cc(C(O)CN)ccc1O, x
epinephrine|epinephrin|adrenaline|adrenalin root root Oc1cc(C(O)CNC)ccc1O, x
adrenalone root root O=C(CNC)c1ccc(O)c(O)c1, x
norephedrine|norephedrin root root
OC(C(, x, N, n,)C), x, c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, Ring, Ring1
ephedrine|ephedrin|pseudoephedrine|pseudoephedrin root root
OC(C(, x, N, n, C)C), x, c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, Ring, Ring1
taurine|taurin root root O, 1@x, S, x, (=O) (=O), x, C, 1, C, 2, N, n
hypotaurine|hypotaurin root root O, 1@x, S, x, (=O), x, C, 1, C, 2, N, n
cadaverine|cadaverin root root N, n, C, 1, C, 2, C, 3, C, 4, C, 5, N, n'
putrescine|putrescin root root N, n, C, 1, C, 2, C, 3, C, 4, N, n'
albizzi aminoacid ine
C, 1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, NC (=O) N, x

alan aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta
homoalan aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | d | delta | w
| omega
alanos aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, N, x, (, x, O, x,)
, x, N, x, =, x, O, x
alloisoleuc aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, [C@H], 2 | a | alpha, Ring, Ring1, [C@@H], 3 | b | beta, (, x,
C, 4 | g | gamma, C, 5 | d | delta,), x, C, 3',
allothreono | allothreon aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, [C@H], 2 | a | alpha, Ring, Ring1, [C@H], 3 | b | beta, (, x, C
, 4 | g | gamma,), x, O, x
allys aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C
, 5 | d | delta, C, 6 | e | epsilon, = O, x
argin aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C
, 5 | d | delta, N, nd | ndelta, C, x, (=, x, N, nw' | nomega',), x, N, nw | nomega | ngamma
asparag aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, (
=, x, O, x,), x, N, ngamma
aspart aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3, C, 4 | g | gamma | b | beta, (
=, x, O, x,), x, O, x
azaser aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, O, x, C (=O) C = [N
+] = [N-], x
betaalan aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nbeta | n3, C, 2 | a | alpha, C, 3 | b | beta, Ring, Ring1
buthion aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, S
, x, CCCC, x
canavan aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, O
NC (=N) N, x
carbocyste aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, S, s, CC (=O), x,
O, 1@x
citrull aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C
, 5 | d | delta, N, x, C, x, (=, x, O, x,), x, N, x
cycloleuc aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, Ring, Ring2, C, 3 | b | beta, C,
4 | g | gamma, C, 5 | d | delta, C, 6, Ring, Ring2
cyste reqineaminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, S, s
cyste aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, S, s, (=O) (=O),
x, O, 1@x,
ethion aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, S
, x, C, x, C, x
isoglutam reqineaminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, Ring, Ring2, ., x, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | bet
a, C, 4 | g | gamma, Ring, Ring2, C, 5 | d | delta, (=, x, O, x,), x, N, x

glutam reqineaminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C, 5 | d | delta, (=, x, O, x,), x, N, nd | ndelta | n5
glutam aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C, 5 | d | delta, (=, x, O, x,), x, O, 1 @ x
glyc aminoacid ine C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1
histid aminoacid ine
C, x, Ring, Ring1, ., x, N, n | nalpha | n2, C, a | alpha, Ring, Ring1, C, b | beta, c, 4, Ring, Ring2, c, 5, n, 1 | nt | ntau | im | nim | n' | tau | prefhydro, c, 2, n, 3 | np | npi, Ring, Ring2
homoargin aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C, 5 | d | delta, C, 6 | e | epsilon, N, nd | ndelta, C, x, (=, x, N, nw' | nomega' ,), x, N, nw | nomega
homocitrull aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C, 5 | d | delta, C, 6 | e | epsilon, N, x, C, x, (=, x, O, x,), x, N, x
homocyste reqineaminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, S, s
homocyste aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, S, s, (=O) (=O), x, O, 1 @ x
homoglutam reqineaminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C, 5 | d | delta, C, 6 | e | epsilon, (=, x, O, x,), x, N, ne | nepsilon | n6
homophenylalan aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, a | alpha, Ring, Ring1, C, b | beta, C, g | gamma, c, x, Ring, Ring2, c, 2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring2
homoprol aminoacid ine
C, x, Ring, Ring1, ., x, N, 1 | n | nalpha | n2, Ring, Ring2, C, 2, Ring, Ring1, C, 3, C, 4, C, 5, C, 6, Ring, Ring2
homoser aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, O, x
homotryptoph aminoacid ane
C, x, Ring, Ring1, ., x, N, n | nalpha | n2, C, a | alpha, Ring, Ring1, C, b | beta, C, g | gamma, C, 3, Ring, Ring2, =, x, C, 2, N, 1, C, 7a, Ring, Ring3, =, x, C, 7, C, 6, =, x, C, 5, C, 4, =, x, C, 3a, Ring, Ring2, Ring, Ring3
iboten aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C2=CC(=O)NO2, x
isoleuc aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, [C@H], 2 | a | alpha, Ring, Ring1, [C@H], 3 | b | beta, (, x, C, 4 | g | gamma, C, 5 | d | delta,), x, C, 3',
isoser aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, Ring, Ring2, ., x, C, 2 | a | alpha, Ring, Ring1, (O), x, C, 3 | b | beta, Ring, Ring2
isoval aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, (, x, C, 2',), x, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma
kynuren aminoacid ine
C, x, Ring, Ring1, ., x, N, n | nalpha | n2, C, a | alpha, Ring, Ring1, C, b | beta, C(=O), x, c, 1, Ring, Ring2, c, 2, (N), x, c, 3, c, 4, c, 5, c, 6, Ring, Ring2
leuc aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, (, x, C, 5 | d | delta,), x, C, 5'

lys aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C
, 5 | d | delta, C, 6 | e | epsilon, N, n6 | nw | nomega | nepsilon | ne | nz | n'
methion aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, S
, x, C, x
mimos aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, N2C=C(O)C(=O)
C=C2, x
norleuc aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C
, 5 | d | delta, C, 6 | e | epsilon
norval aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C
, 5 | d | delta
ornith aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C
, 5 | d | delta, N, n5 | ndelta | nd
penicillam aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, (C) (C) S, x
phenylalan|3phenylalan|betaphenylalan aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, a | alpha, Ring, Ring1, C, b | beta, c, x, Ring, Ring2, c,
2 | o | ortho, c, 3 | m | meta, c, 4 | p | para, c, 5, c, 6, Ring, Ring2
prol aminoacid ine
C, x, Ring, Ring1, ., x, N, 1 | n | nalpha | n2, Ring, Ring2, C, 2, Ring, Ring1, C, 3, C, 4, C, 5, Ring, Ri
ng2
3hydroxyprol|hydroxyprol aminoacid ine
C, x, Ring, Ring1, ., x, N, 1 | n | nalpha | n2, Ring, Ring2, C, 2, Ring, Ring1, C, 3, (O), x, C, 4, C, 5, R
ing, Ring2
4hydroxyprol aminoacid ine
C, x, Ring, Ring1, ., x, N, 1 | n | nalpha | n2, Ring, Ring2, C, 2, Ring, Ring1, C, 3, C, 4, (O), x, C, 5, R
ing, Ring2
5hydroxyprol aminoacid ine
C, x, Ring, Ring1, ., x, N, 1 | n | nalpha | n2, Ring, Ring2, C, 2, Ring, Ring1, C, 3, C, 4, C, 5, (O), x, R
ing, Ring2
pyroglutam aminoacid ine
C, x, Ring, Ring1, ., x, N, 1 | n | nalpha | n2, Ring, Ring2, C, 2, Ring, Ring1, C, 3, C, 4, C, 5, (=O), x,
Ring, Ring2
sarcos aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, (, x, C, 2 | a | alpha, Ring, Ring1,), x, C, x
selenocyste reqineaminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, [Se], se
selenomethion aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, [
Se], x, C, x
ser aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, O, x
tleuc|tertleuc aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, (, x, C, 3',) (, x
, C, 3'',), x, C, 3'''
theano|thean aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C
, x, (=O), x, N, x, C, x, C, x
thiocitrull aminoacid ine
C,1, Ring, Ring1, ., x, N, n | nalpha | n2, C, 2 | a | alpha, Ring, Ring1, C, 3 | b | beta, C, 4 | g | gamma, C
, 5 | d | delta, N, x, C, x, (=, x, S, x,), x, N, x

[illegible]

•

x

mannosamine|mannosamin sugar trivial

O,x,=,x,C,1,[C@@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,6,O,x

fucosamine|fucosamin sugar trivial

O,x,=,x,C,1,[C@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@@H](,4,O,x,)[C@H](,5,O,x,),x,C,6

quinovosamine|quinovosamin sugar trivial

O,x,=,x,C,1,[C@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,6

rhamnosamine|rhamnosamin sugar trivial

O,x,=,x,C,1,[C@@H](,2,N,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,6

glucal sugar trivial

C,1,Ring,Ring1,=,x,C,2,[C@@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O1),x,C,6,O,x

rhamnal sugar trivial

C,1,Ring,Ring1,=,x,C,2,[C@@H],3,(O),x,[C@H],4,(O),x,[C@H],5,(O1),x,C,6

galactal sugar trivial

C,1,Ring,Ring1,=,x,C,2,[C@@H],3,(O),x,[C@@H],4,(O),x,[C@H],5,(O1),x,C,6,O,x

glucamine sugar trivial

N,n,C,1,[C@H](,2,O,x,),x,[C@@H](,3,O,x,),x,[C@H](,4,O,x,)[C@H](,5,O,x,),x,C,6,O,x

sucr sugar disugar

OC[C@@]1([C@@H](O)[C@H](O)[C@H](O1)CO)O[C@@H]2[C@H](O)[C@@H](O)[C@H](O)[C@@H](CO)O2,x

trehal sugar disugar

O[C@H]1[C@H](O)[C@@H](CO)O[C@H](O[C@H]2[C@@H](O)[C@H](O)[C@@H](O)[C@H](CO)O2)[C@@H]1O,x

melezit sugar disugar

OC[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)[C@@H](O[C@@]2(CO)[C@@H](O[C@H]3O[C@H](CO)[C@@H](O)[C@H](O)[C@H]3O)[C@H](O)[C@@H](CO)O2)O1,x

stachy|lupe sugar disugar

O[C@H]1[C@@H](CO)O[C@H](OC[C@H]2O[C@H](O[C@H]3[C@@H](O[C@]4(CO)O[C@H](CO)[C@@H](O)[C@@H]4O)O[C@H](CO)[C@@H](O)[C@@H]3O)[C@H](O)[C@@H](O)[C@H]2O)[C@H](O)[C@H]1O,x

lact sugar disugar

OC[C@H]1O[C@@H](O[C@@H]([C@H](O)[C@@H](O)[C@@H](O)O2)[C@H]2CO)[C@H](O)[C@@H](O)[C@H]1O,x

malt|maltobi sugar disugar

O[C@@H]1[C@@H](O)[C@@H](O[C@H]2[C@H](O)[C@@H](O)[C@@H](O)O[C@@H]2CO)O[C@H](CO)[C@@H]1O,x

maltotri sugar disugar

O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CO)O[C@@H]1O[C@@H]2[C@@H](CO)O[C@H](O[C@@H]3[C@@H](CO)OC(O)[C@H](O)[C@H]3O)[C@H](O)[C@H]2O,x

maltotetra sugar disugar

O[C@@H]([C@@H](O[C@H]4[C@H](O)[C@H]([C@@H](O)O[C@@H]4CO)O)O[C@@H]1CO)[C@@H](O)[C@@H]1O[C@@H]2[C@H](O)[C@H]([C@H](O[C@@H](O[C@H](CO)[C@H]3O)[C@H](O)[C@H]3O)[C@@H](CO)O2)O,x

maltopenta sugar disugar

O[C@H]([C@H]2O)[C@H](O[C@H](CO)[C@H]2O)O[C@@H]1[C@@H](CO)O[C@H](O[C@H]3[C@H](O)[C@H]([C@@H](O[C@H]4[C@H](O)[C@H]([C@@H](O[C@H]5[C@H](O)[C@H]([C@@H](O)O[C@@H]5CO)O)O[C@@H]4CO)O)O[C@@H]3CO)O)[C@H](O)[C@H]1O,x

maltohexa sugar disugar

O[C@@H]([C@@H](O[C@H]3[C@H](O)[C@H]([C@@H](O[C@H]6[C@H](O)[C@H]([C@@H](O)O[C@@H]6CO)O)O[C@@H]3CO)O)O[C@@H]1CO)[C@@H](O)[C@@H]1O[C@@H]2[C@H](O)[C@H]([C@H](O[C@@H]4[C@H](O)[C@H]([C@H](O[C@@H](O[C@H](CO)[C@H]5O)[C@H](O)[C@H]5O)[C@@H](CO)O4)O)[C@@H](CO)O2)O,x

inositol pseudosugar unknown x,x
 inositol root root OC1C(O)C(O)C(O)C(O)C1O,x
 mesoinositol|myoinositol root root
 O,x,[C@H],1, Ring, Ring1, [C@@H],2,(O),x,[C@@H],3,(O),x,[C@H],4,(O),x,[C@@H],5,(O),
 x,[C@@H],6, Ring, Ring1, O,x
 scylloinositol root root
 O,x,[C@H],1, Ring, Ring1, [C@H],2,(O),x,[C@@H],3,(O),x,[C@H],4,(O),x,[C@@H],5,(O),x,
 [C@@H],6, Ring, Ring1, O,x
 epiinositol root root
 O,x,[C@H],1, Ring, Ring1, [C@@H],2,(O),x,[C@@H],3,(O),x,[C@@H],4,(O),x,[C@@H],5,(O)
 x,[C@@H],6, Ring, Ring1, O,x
 dinositol root root O[C@H]1[C@@H](O)[C@H](O)[C@H](O)[C@@H](O)[C@@H]1O,x
 linositol root root O[C@@H]1[C@H](O)[C@@H](O)[C@@H](O)[C@H](O)[C@H]1O,x
 quebrachitol root root O[C@@H]1[C@H](O)[C@@H](O)[C@@H](OC)[C@H](O)[C@H]1O,x
 muram pseudosugar unknown x,x
 muram root root
 CC(C)O,x,[C@H],3, Ring, Ring1, [C@H],4,(O),x,[C@@H],5,(x,C,6,O,x),x,O,x,[C@H],1,(
 O),x,[C@H],2,(x,N,n),x, Ring, Ring1
 neuramin pseudosugar unknown x,x
 neuramin root root
 C,x,[C@@],2, Ring, Ring1, (O),x,O,x,[C@@H],6,(x,[C@H],7,(O),x,[C@H],8,(O),x,C,9,O,
 x),x,[C@H],5,(x,N,n),x,[C@@H],4,(O),x,C,3, Ring, Ring1
 sial pseudosugar unknown x,x
 sial root root
 C,x,[C@@],2, Ring, Ring1, (O),x,O,x,[C@@H],6,(x,[C@H],7,(O),x,[C@H],8,(O),x,C,9,O,
 x),x,[C@H],5,(x,NC(=O)C,x),x,[C@@H],4,(O),x,C,3, Ring, Ring1

 adenos|adenyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6,(x,N,n|n6,) ,x,n,1,c,2,n,3
 ,c,4, Ring, Ring3, Ring, Ring2
 cytid|cytidyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,1, Ring, Ring2, c,2,(=O),x,n,3,c,4,(x,N,n|n4,) ,x,c,5,c,6, Ring, Ring2
 guanos|guanyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6,(=O),x,N,1,c,2,(x,N,n|n2,
) ,x,n,3,c,4, Ring, Ring3, Ring, Ring2
 inos nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6,(O),x,n,1,c,2,n,3,c,4, Ring
 , Ring3, Ring, Ring2
 thymid|thymidyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,C,2', [C@@H],1', (O,x, Ring, Ring1,) ,x
 ,n,1, Ring, Ring2, c,2,(=O),x,n,3|n,c,4,(=O),x,c,5,(C),x,c,6, Ring, Ring2
 urid|uridyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,1, Ring, Ring2, c,2,(=O),x,n,3|n,c,4,(=O),x,c,5,c,6, Ring, Ring2
 xanthos|xanthoyl|xanthonyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,9, Ring, Ring2, c,8,n,7,c,5, Ring, Ring3, c,6,(O),x,n,1,c,2,(O),x,n,3,c,
 4, Ring, Ring3, Ring, Ring2
 orotid|orotidyl nucleotide nucleotide
 O,x,C,5', [C@@H],4', Ring, Ring1, [C@@H],3', (O),x,[C@@H],2', (O),x,[C@@H],1', (O,x,Rin
 g, Ring1,) ,x,n,1, Ring, Ring2, c,2,(=O),x,n,3,c,4,(=O),x,c,5,c,6,(C(=O)O),x, Ring, Rin
 g2

[illegible]

adenyl loveracid root

cytidyl loveracid root

quanyl loveracid root

```

inos loveracid root

```

thymidyl loveracid root

uridyl loveracid root

xanthoyl | xanthonyl loveracid root

purineriboside root root

thuj root root

car root root

norcar root root

```
C,2, Ring, Ring1, (, x, C, 10, ) , x, C, 3, C, 4, C, 5, (, x, C, 7, Ring, Ring2, ) , x, C, 6, (, x, C, 8, ) (, x, C, 9, ) . x, C, 1, Ring, Ring2, Ring, Ring1
```

norpin root root

```
C, 2, Ring, Ring1, C, 3, C, 4, C, 5, (, x, C, 7, Ring, Ring2, ), x, C, 6, C, 1, Ring, Ring2, Ring, Ring1
```

camphor loveracid root

```
C,10,C,1, Ring, Ring1, Ring, Ring2, C,2,C,3,C,4, (,x,C,5,C,6, Ring, Ring1,) ,x,C,7, (,x,C,8,) ,x, (,x,C,9,) ,x, Ring, Ring2
```

camphor root root

```
C,10,C,1, Ring, Ring1, Ring, Ring2, C, 2, (=0), x, C, 3, C, 4, (, x, C, 5, C, 6, Ring, Ring1, ), x, C, 7, (, x, C, 8, ), x, (, x, C, 9, ), x, Ring, Ring2
```

[illegible]

farnes root root
C,1,C,2,=,x,C,3,(C),x,C,4,C,5,C,6,=,x,C,7,(C),x,C,8,C,9,C,10,=,x,C,11,(C)C,x
ocimene root root C,1,=,x,C,2,C,3,(C)=,x,C,4,C,5,C,6,=,x,C,7,(C),x,C,8
alloocimene|allocimen root root
C,1,C,2,(C)=,x,C,3,C,4,=,x,C,5,(C),x,C,6,=,x,C,7,C,8
nerolid root root C(C)(C=C)CCC=C(C)CCC=C(C)C,x
all root root C,1|a|alpha,C,2|b|beta,=,x,C,3|g|gamma
isoall root root C,1|a|alpha,=,x,C,2|b|beta,C,3|g|gamma
homoall root root C,1|a|alpha,C,2|b|beta,C,3|g|gamma,=,x,C,4|d|delta
methall root root C,1,C,2,(,x,C,x,)x,=,x,C,3
triazeno root root N,4@1,=,x,N,2,N,3
vin root root C,1|a|alpha,=,x,C,2|b|beta
hydrazine|hydrazin root root N,1|n,N,2|n'
dithioiminocarbonate root root S,1@s,C,x,(=,x,N,n,)x,S,1@s'
urea|carbamide|carbamid root root N,1|n,C,2,(,x,=,x,O,o,)x,N,3|n'
sulfocarbamide|sulfocarbamid|sulfoarea root root
N,1|n,C,2,(,x,=,x,S,s,)x,N,3|n'
biurea root root N,1,C,2,(=O),x,N,3,N,4,C,5,(=O),x,N,6
guanyl root root C,4@x,(=N),x,N,x
uronium root root N,1|n,C,2,(,x,N,3|n',),x,=,x,[O+],o
ureido root root N,4@1|n,C,2,(,x,=,x,O,o,)x,N,3|n'
ureylene|ureylen root bridge N,4@1|n,C,2,(,x,=,x,O,o,)x,N,4@3|n'
carbanilide|carbanilid root root
c,6,ring,ring1,c,5,c,4,c,3,c,2,c,1,ring,ring1,N,n,C,x,(,x,=,x,O,o,)x,N,n',c,1',
ring,ring2,c,2',c,3',c,4',c,5',c,6',ring,ring2
tms root root [Si],4@x,(C)(C)(C),x
tbds root root [Si],4@x,(C(C)(C)C)(C)(C),x
plumb root root [Pb],1
sil root root [Si],x
stann root root [Sn],x
bor root root [B],x
germ root root [Ge],x
amine|amin|ammonia root root N,n
phosphine|phosphin root root P,x
arsine|arsin root root [As],x
hydrogen root root [H],4@x
deuterium root root [2H],4@x
tritium root root [3H],4@x
hydrido root root [H-],4@x
deuterido root root [2H-],4@x
lithio root root [Li],4@x
sodio root root [Na],4@x
potassio|kalio root root [K],4@x
fluoro|fluor root root F,4@x
chloro|chlor root root Cl,4@x
chlorosyl root root Cl,4@x,=O,x
chloryl root root Cl,4@x,(=O)=O,x
perchloryl root root Cl,4@x,(=O)(=O)=O,x
borono root root [B],4@x,(O)O,x
lithium root metal [Li],x
sodium|natrium root metal [Na],x
potassium|kalium root metal [K],x
rubidium root metal [Rb],x
cesium root metal [Cs],x
francium root metal [Fr],x
beryllium|glucinium root metal [Be],x
magnesium root metal [Mg],x

calcium root metal [Ca],x
strontium root metal [Sr],x
barium root metal [Ba],x
radium root metal [Ra],x
scandium root metal [Sc],x
yttrium root metal [Y],x
lanthanum root metal [La],x
cerium root metal [Ce],x
praesodymium|praseodymium root metal [Pr],x
neodymium root metal [Nd],x
promethium root metal [Pm],x
samarium root metal [Sm],x
europium root metal [Eu],x
gadolinium root metal [Gd],x
terbium root metal [Tb],x
dysprosium root metal [Dy],x
holmium root metal [Ho],x
erbium root metal [Er],x
thulium root metal [Tm],x
ytterbium root metal [Yb],x
lutetium|cassiopeium root metal [Lu],x
actinium root metal [Ac],x
thorium root metal [Th],x
protactinium root metal [Pa],x
uranium root metal [U],x
neptunium root metal [Np],x
plutonium root metal [Pu],x
americium root metal [Am],x
curium root metal [Cm],x
berkelium root metal [Bk],x
californium root metal [Cf],x
einsteinium root metal [Es],x
fermium root metal [Fm],x
mendelevium root metal [Md],x
nobelium root metal [No],x
lawrencium root metal [Lr],x
titanium root metal [Ti],x
zirconium root metal [Zr],x
hafnium root metal [Hf],x
vanadium root metal [V],x
niobium root metal [Nb],x
tantalum root metal [Ta],x
chromium root metal [Cr],x
molybdenum root metal [Mo],x
tungsten root metal [W],x
manganese root metal [Mn],x
technetium root metal [Tc],x
rhenium root metal [Re],x
iron root metal [Fe],x
ruthenium root metal [Ru],x
osmium root metal [Os],x
cobalt root metal [Co],x
rhodium root metal [Rh],x
iridium root metal [Ir],x
nickel root metal [Ni],x
palladium root metal [Pd],x
platinum root metal [Pt],x

[illegible]

```

cresolindphenol root root
O,x,=,x,C,1, Ring, Ring1, C,2,=,x,C,3,C,4,(,x,C,5,=,x,C,6, Ring, Ring1, ),x,=,x,N,x,C,
1', Ring, Ring2, =,x,C,2' |m| meta, (C), x,C,3' |o| ortho, =,x,C,4', (,x,O,x, ), x,C,5', =,x,C,
,6', Ring, Ring2
picoline|picolin|picol toluene picoline
c,2, Ring, Ring1, c,3 |b| beta, c,4 |g| gamma, c,5, c,6, n,1, Ring, Ring1
pipecoline|pipecolin|pipecol toluene picoline
C,2 |a| alpha, Ring, Ring1, C,3 |b| beta, C,4 |g| gamma |p, C,5, C,6, N,1, Ring, Ring1
toluene|tolu|tol toluene toluene
c,1, Ring, Ring1, c,2 |o| ortho, Ring, Ring2, ., x, c,4 |p| para, Ring, Ring3, Ring, Ring4, ., x, c
,6, Ring, Ring5, Ring, Ring1, ., x, c,3 |m| meta, Ring, Ring2, Ring, Ring3, ., x, c,5, Ring, Ring4
, Ring, Ring5
toluidide|otoluidide|toluide|otoluide toluidide toluene
O,8@x, ., x, N,4@x, c,1', Ring, Ring1, c,2' |o| ortho, c,3' |m| meta, c,4' |p| para, c,5', c,6', R
ing, Ring1
cumidine|cumidin toluene cumene
N,n,c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, =,x, c,6, Ring, Ring1
cumene|cumen toluene cumene
c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, =,x, c,6, Ring, Ring1
cumyl|alphacumyl root root
C,4@a|alpha, (C) (C), x, c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,6, Ring, Ring1
cumidene|cumiden toluene cumene
N,n,c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, =,x, c,6, Ring, Ring1
cymene|cymen toluene cymene
C,7 |a| alpha, c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
xylene|xylol toluene toluene
C,a|alpha, c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
xylen|xyl toluene xylidine
c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
xylidide|oxylidide|xylide|oxylide toluidide xylidine
O,8@x, ., x, N,4@x, c,1', Ring, Ring1, c,2' |o| ortho, c,3' |m| meta, c,4' |p| para, c,5', c,6', R
ing, Ring1
anis toluene anisidine
c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
thioanis toluene thioanisidine
c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
homoanis toluene anisidine
C,x,C,x,c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
anisidide|oanisidide|anisode|oanisode toluidide anisidine
O,8@x, ., x, N,4@x, c,1', Ring, Ring1, c,2' |o| ortho, c,3' |m| meta, c,4' |p| para, c,5', c,6', R
ing, Ring1
anisal toluene anisidine
C,8@x, c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
mentha|menth|neomenth|neomentha|isomenth|isomentha toluene cymene
C,3 |m| meta, Ring, Ring1, C,4 |p| para, C,5, C,6, C,1, Ring, Ring2, C,2 |o| ortho, Ring, Ring1, .
,x, C,7 |a| alpha, Ring, Ring2
anisidine|anisidin toluene anisidine
N,n,c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
anisidino toluene anisidine
N,4@n, c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
phenetidine|phenetidin toluene phenetidine
N,n,c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1
phenetidide|ophenetidide|phenetide|ophenetide toluidide phenetidine
O,8@x, ., x, N,4@x, c,1', Ring, Ring1, c,2' |o| ortho, c,3' |m| meta, c,4' |p| para, c,5', c,6', R
ing, Ring1
phenetidino toluene phenetidine
N,4@n, c,1, Ring, Ring1, c,2 |o| ortho, c,3 |m| meta, c,4 |p| para, c,5, c,6, Ring, Ring1

```

[illegible]

[illegible]

Figure 1: Schematic representation of the 12 genes and their expression patterns in the developing mouse embryo. The figure shows 12 genes (A-L) and their expression patterns in the developing mouse embryo. The genes are: A) HNF1A, B) HNF1B, C) HNF1C, D) HNF1D, E) HNF1E, F) HNF1F, G) HNF1G, H) HNF1H, I) HNF1I, J) HNF1J, K) HNF1K, L) HNF1L. The expression patterns are shown as black bars indicating the expression of each gene in different tissues and developmental stages.

Region	1990	1991	1992	1993	1994	1995	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014	2015	2016	2017	2018	2019	2020	2021	2022	2023	2024	2025	2026	2027	2028	2029	2030	2031	2032	2033	2034	2035	2036	2037	2038	2039	2040	2041	2042	2043	2044	2045	2046	2047	2048	2049	2050	2051	2052	2053	2054	2055	2056	2057	2058	2059	2060	2061	2062	2063	2064	2065	2066	2067	2068	2069	2070	2071	2072	2073	2074	2075	2076	2077	2078	2079	2080	2081	2082	2083	2084	2085	2086	2087	2088	2089	2090	2091	2092	2093	2094	2095	2096	2097	2098	2099	2100																																																																																																																																																																																																	
North America	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2.0	2.1	2.2	2.3	2.4	2.5	2.6	2.7	2.8	2.9	3.0	3.1	3.2	3.3	3.4	3.5	3.6	3.7	3.8	3.9	4.0	4.1	4.2	4.3	4.4	4.5	4.6	4.7	4.8	4.9	5.0	5.1	5.2	5.3	5.4	5.5	5.6	5.7	5.8	5.9	6.0	6.1	6.2	6.3	6.4	6.5	6.6	6.7	6.8	6.9	7.0	7.1	7.2	7.3	7.4	7.5	7.6	7.7	7.8	7.9	8.0	8.1	8.2	8.3	8.4	8.5	8.6	8.7	8.8	8.9	9.0	9.1	9.2	9.3	9.4	9.5	9.6	9.7	9.8	9.9	10.0	10.1	10.2	10.3	10.4	10.5	10.6	10.7	10.8	10.9	11.0	11.1	11.2	11.3	11.4	11.5	11.6	11.7	11.8	11.9	12.0	12.1	12.2	12.3	12.4	12.5	12.6	12.7	12.8	12.9	13.0	13.1	13.2	13.3	13.4	13.5	13.6	13.7	13.8	13.9	14.0	14.1	14.2	14.3	14.4	14.5	14.6	14.7	14.8	14.9	15.0	15.1	15.2	15.3	15.4	15.5	15.6	15.7	15.8	15.9	16.0	16.1	16.2	16.3	16.4	16.5	16.6	16.7	16.8	16.9	17.0	17.1	17.2	17.3	17.4	17.5	17.6	17.7	17.8	17.9	18.0	18.1	18.2	18.3	18.4	18.5	18.6	18.7	18.8	18.9	19.0	19.1	19.2	19.3	19.4	19.5	19.6	19.7	19.8	19.9	20.0	20.1	20.2	20.3	20.4	20.5	20.6	20.7	20.8	20.9	21.0	21.1	21.2	21.3	21.4	21.5	21.6	21.7	21.8	21.9	22.0	22.1	22.2	22.3	22.4	22.5	22.6	22.7	22.8	22.9	23.0	23.1	23.2	23.3	23.4	23.5	23.6	23.7	23.8	23.9	24.0	24.1	24.2	24.3	24.4	24.5	24.6	24.7	24.8	24.9	25.0	25.1	25.2	25.3	25.4	25.5	25.6	25.7	25.8	25.9	26.0	26.1	26.2	26.3	26.4	26.5	26.6	26.7	26.8	26.9	27.0	27.1	27.2	27.3	27.4	27.5	27.6	27.7	27.8	27.9	28.0	28.1	28.2	28.3	28.4	28.5	28.6	28.7	28.8	28.9	29.0	29.1	29.2	29.3	29.4	29.5	29.6	29.7	29.8	29.9	30.0	30.1	30.2	30.3	30.4	30.5	30.6	30.7	30.8	30.9	31.0	31.1	31.2	31.3	31.4	3

[illegible]

[illegible]

[illegible]

```

pyranthrene|pyranthren root root
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 4b, Ring, Ring3, c, 5, c, 5a, Ring, Ring4, c, 6, c, 7, c, 7a, Ring, Ring5, c, 8, c, 8a, Ring, Ring6, c, 9, c, 10, c, 11, c, 12, c, 12a, Ring, Ring6, c, 12b, Ring, Ring7, c, 13, c, 13a, Ring, Ring8, c, 14, c, 15, c, 15a, (, x, c, 16, c, 16a, Ring, Ring2, Ring, Ring1, ), x, c, 15b, Ring, Ring3, c, 15c, Ring, Ring8, c, 15d, Ring, Ring4, c, 15e, Ring, Ring7, Ring, Ring5
ovalene|ovalen root root
c,1, Ring, Ring1, c, 2, c, 2a, Ring, Ring2, c, 3, c, 4, c, 4a, Ring, Ring3, c, 5, c, 6, c, 6a, Ring, Ring4, c, 7, c, 7a, Ring, Ring5, c, 8, c, 9, c, 9a, Ring, Ring6, c, 10, c, 11, c, 11a, Ring, Ring7, c, 12, c, 13, c, 13a, Ring, Ring8, c, 14, c, 14a, Ring, Ring1, c, 14b, Ring, Ring9, c, 14c, Ring, Ring2, c, 14d, Ring, Ring3, c, 14e, Ring, Ring4, c, 14f, Ring, Ring0, c, 14g, Ring, Ring5, c, 14h, Ring, Ring6, c, 14i, Ring, Ring7, c, 14j, Ring, Ring8, c, 14k, Ring, Ring0, Ring, Ring9
biphenylene|biphenylen root root
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 4b, Ring, Ring3, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring3, c, 8b, Ring, Ring2, Ring, Ring1
thianthrene|thianthren root root
c,1, Ring, Ring1, c, 2, c, 3, c, 4, c, 4a, Ring, Ring2, s, 5, c, 5a, Ring, Ring3, c, 6, c, 7, c, 8, c, 9, c, 9a, Ring, Ring3, s, 10, c, 10a, Ring, Ring2, Ring, Ring1
pyr root root
c,2|a|alpha, Ring, Ring1, c, 3|b|beta, c, 4|g|gamma, c, 5, c, 6, o, 1, Ring, Ring1
pyrano opfuser unknown c,2, Ring, Ring1, c, 3, c, 4, c, 5, c, 6, o, 1, Ring, Ring1
mdioxine|mdioxin root root c,2, Ring, Ring1, o, 3, c, 4, c, 5, c, 6, o, 1, Ring, Ring1
pdioxine|pdioxin root root c,2, Ring, Ring1, c, 3, o, 4, c, 5, c, 6, o, 1, Ring, Ring1
oxalene|oxalen root root
c,1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, o, 7, c, 7a, Ring, Ring2, Ring, Ring1
azalene|azalen root root
c,1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, n, 7, c, 7a, Ring, Ring2, Ring, Ring1
isobenzofuran root root
c,1, Ring, Ring1, o, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring2, Ring, Ring1
benzofurazan root root
n,1, Ring, Ring1, o, 2, n, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring2, Ring, Ring1
benzofuroxan root root [n+], 1, (, x, [O-], x, ), x, Ring, Ring1, o, 2, n, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring2, Ring, Ring1
piazhthiole root root
n,1, Ring, Ring1, s, 2, n, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring2, Ring, Ring1
catecholborane root root
o, x, Ring, Ring1, B, b, O, x, c, 2, Ring, Ring2, c, 3, c, 4, c, 5, c, 6, c, 1, Ring, Ring2, Ring, Ring1
chromene|chromen root root
c,2, Ring, Ring1, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1
chromane|chroman root root
C,2, Ring, Ring1, C,3, C,4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring2, O, 1, Ring, Ring1
chromone|chromon root root
c,2, Ring, Ring1, c, 3, c, 4, (=O), x, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1
esculetin root root
c,2, Ring, Ring1, (=O), x, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, (O), x, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1

```

```

umbelliferone root root
c,2, Ring, Ring1, (=O), x, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1
umbelliferoyl root root
c,2, Ring, Ring1, (=O), x, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 4@7, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1
isochromane|isochroman root root
C, 1, Ring, Ring1, O, 2, C, 3, C, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
flav root root C, 2|a-t, (, x, Ring, Ring1, C, 3|a-b, C, 4|a-
1, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring2, O, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring3
flavone|flavon root root c, 2|a-t, (, x, Ring, Ring1, c, 3|a-b, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring3
acacetin root root c, 2|a-t, (, x, Ring, Ring1, c, 3|a-b, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', c, 4', (OC), x, c, 5', c, 6', Ring, Ring3
alpinetin root root C, 2|a-t, (, x, Ring, Ring1, C, 3|a-b, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, (OC), x, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring3
apigenin root root c, 2|a-t, (, x, Ring, Ring1, c, 3|a-b, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', c, 4', (O), x, c, 5', c, 6', Ring, Ring3
baicalein root root c, 2|a-t, (, x, Ring, Ring1, c, 3|a-b, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, (O), x, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring3
catechin root root C, 2|a-t, (, x, Ring, Ring1, C, 3|a-b, (O), x, C, 4|a-
1, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, O, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', (O), x, c, 4', (O), x, c, 5', c, 6', Ring, Ring3
chrysin root root c, 2|a-t, (, x, Ring, Ring1, c, 3|a-b, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', (OC), x, c, 4', (O), x, c, 5', (OC), x, c, 6', Ring, Ring3
cirsiliol root root c, 2|a-t, (, x, Ring, Ring1, c, 3|a-b, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, (OC), x, c, 7, (OC), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', (O), x, c, 4', (O), x, c, 5', c, 6', Ring, Ring3
diosmetin root root c, 2|a-t, (, x, Ring, Ring1, c, 3|a-b, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', (O), x, c, 4', (OC), x, c, 5', c, 6', Ring, Ring3
epicatechin root root C, 2|a-t, (, x, Ring, Ring1, C, 3|a-b, (O), x, C, 4|a-
1, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', (O), x, c, 4', (O), x, c, 5', c, 6', Ring, Ring3
eupatorin root root c, 2|a-t, (, x, Ring, Ring1, c, 3|a-b, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, (OC), x, c, 7, (OC), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', (O), x, c, 4', (OC), x, c, 5', c, 6', Ring, Ring3
galangin root root c, 2|a-t, (, x, Ring, Ring1, c, 3|a-b, (O), x, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring3
genkwanin root root c, 2|a-t, (, x, Ring, Ring1, c, 3|a-b, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, c, 7, (OC), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', c, 4', (O), x, c, 5', c, 6', Ring, Ring3
hesperitin root root c, 2|a-t, (, x, Ring, Ring1, c, 3|a-b, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', (O), x, c, 4', (OC), x, c, 5', c, 6', Ring, Ring3
kaempferide|kaempferol root root c, 2|a-t, (, x, Ring, Ring1, c, 3|a-b, (O), x, c, 4|a-
1, (=O), x, c, 4a, Ring, Ring2, c, 5, (O), x, c, 6, c, 7, (O), x, c, 8, c, 8a, Ring, Ring2, o, 1, Ring, Ring1, ), x, c, 1', Ring, Ring3, c, 2', c, 3', c, 4', (O), x, c, 5', c, 6', Ring, Ring3

```


[illegible]

phenothiasilin root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, S, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, [Si], 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenothiagermanin root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, S, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, [Ge], 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenaz root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, n, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, n, 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenazasilin|phenazasilin root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, N, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, [Si], 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenarsaz|phenoarsaz root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, n, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, [as], 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenothiaz|thiodiphenylamine root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, s, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, n, 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenomercaz root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, N, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, [Hg], 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenophosphaz root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, n, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, p, 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenotelluraz root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, [Te], 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,
 9, c, 9a, Ring, Ring3, N, 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenoselenaz root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, [Se], 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,
 9, c, 9a, Ring, Ring3, N, 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenothiars root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, s, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, [as], 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenoxantimon root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, O, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, [Sb], 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenoxars root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, o, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, [as], 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenoxaphos root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, O, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, P, 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenoxatellur root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, O, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, [Te], 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenoxaselen root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, O, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, [Se], 10, c, 10a, Ring, Ring2, Ring, Ring1
 dibenzodioxin root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, o, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, o, 10, c, 10a, Ring, Ring2, Ring, Ring1
 phenoxaz|phenazox root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,4a, Ring, Ring2, o, 5, c, 5a, Ring, Ring3, c,6, c,7, c,8, c,9, c
 ,9a, Ring, Ring3, n, 10, c, 10a, Ring, Ring2, Ring, Ring1
 indene|inden root root
 c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
 2

```

indeno opfuser unknown
c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
indole|indol root root
n,1, Ring, Ring1, c,2 |a|alpha, c,3 |b|beta, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring,
Ring1, Ring, Ring2
thianaphthene|thianaphthen|thionaphthene|thionaphthen root root
s,1, Ring, Ring1, c,2 |a|alpha, c,3 |b|beta, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring,
Ring1, Ring, Ring2
thianaphtheno|thianaphthen opfuser unknown
s,1, Ring, Ring1, c,2 |a|alpha, c,3 |b|beta, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring,
Ring1, Ring, Ring2
isothianaphthene|isothianaphthen root root
c,1, Ring, Ring1, s,2 |a|alpha, c,3 |b|beta, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring,
Ring1, Ring, Ring2
isothianaphtheno|isothianaphthen opfuser unknown
c,1, Ring, Ring1, s,2 |a|alpha, c,3 |b|beta, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring,
Ring1, Ring, Ring2
skatole|skatol root root
n,1, Ring, Ring1, c,2, c,3, (C), x, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Rin
g, Ring2
gramine root root
n,1, Ring, Ring1, c,2, c,3, (CN(C)C), x, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring
1, Ring, Ring2
indolo opfuser unknown
n,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
isoindole|isoindol root root
c,1, Ring, Ring1, n,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
isoindolo opfuser unknown
c,1, Ring, Ring1, n,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
arsindole|arsindol root root
[as], 1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, R
ing2
arsindolo opfuser unknown
[as], 1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, R
ing2
isoarsindole|isoarsindol root root
c,1, Ring, Ring1, [as], 2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, R
ing2
isoarsindolo|isoarsindol opfuser unknown
c,1, Ring, Ring1, [as], 2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, R
ing2
phosphindole|arsindol root root
p,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
phosphindolo|arsindol opfuser unknown
p,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
isophosphindole|isoarsindol root root
c,1, Ring, Ring1, p,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2
isophosphindolo|isoarsindol opfuser unknown
c,1, Ring, Ring1, p,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring
2

```

indazole|indazol root root
n,1, Ring, Ring1, n,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
indazolo|indazol opfuser unknown
n,1, Ring, Ring1, n,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
indolizine|indolizin|pyrrocol root root
c,1, Ring, Ring1, c,2, c,3, n,4, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
indolizino opfuser unknown
c,1, Ring, Ring1, c,2, c,3, n,4, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
oxindole|oxindol root root
N,1, Ring, Ring1, C,2, (=, x, O, x,), x, C,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
indoline|indolin root root
N,1, Ring, Ring1, C,2, C,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
isat root root
N,1, Ring, Ring1, C,2|alpha, (=O), x, C,3|beta, (=O), x, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
isoindoline|isoindolin root root
C,1, Ring, Ring1, N,2, C,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
indane|indan|hydrindene|hydrind root root
C,1|a|alpha, Ring, Ring1, C,2|b|beta, C,3, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
hydrindantin root root O=C(c2c1cccc2)C(C1=O)(O)C(C3=O)(O)C(c4c3cccc4)=O, x
alloxantin root root OC1(C2(C(NC(NC2=O)=O)=O)O)C(NC(NC1=O)=O)=O, x
ninhydrin root root
C,1, (=O), x, Ring, Ring1, C,2, (=O), x, C,3, (=O), x, c,3a, Ring, Ring2, c,4, c,5, c,6, c,7, c,7a, Ring, Ring1, Ring, Ring2
tetral root root
C,1|a|alpha, Ring, Ring1, C,2|b|beta, C,3, C,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
decal root root
C,1|a|alpha, Ring, Ring1, C,2|b|beta, C,3, C,4, C,10, Ring, Ring2, C,5, C,6, C,7, C,8, C,9, Ring, Ring1, Ring, Ring2
hexalin root root C,1, Ring, Ring1, C,2, C,3, C,4, C,5, C,6, Ring, Ring1
quinol|chinol|quinolin|chinolin|leucol root root
n,1, Ring, Ring1, c,2|b|beta, c,3, c,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
quinolin|chinolin opfuser unknown
n,1, Ring, Ring1, c,2|b|beta, c,3, c,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
carbostyryl|carbostyryl root root
n,1, Ring, Ring1, c,2|b|beta, (O), x, c,3, c,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
isocarbostyryl|isocarbostyryl root root
c,1, (O), x, Ring, Ring1, n,2|b|beta, c,3, c,4, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
lepid root root
n,1, Ring, Ring1, c,2|b|beta, c,3, c,4, (C), x, c,4a, Ring, Ring2, c,5, c,6, c,7, c,8, c,8a, Ring, Ring1, Ring, Ring2
cinchonin loveracid root
c,4, Ring, Ring1, c,3, c,2, n,1, c,8a, Ring, Ring2, c,8, c,7, c,6, c,5, c,4a, Ring, Ring1, Ring, Ring2

[illegible]

Variable	Mean	SD	Min	Max	Median	Q1	Q3	Mode	Skewness	Kurtosis	Shapiro-Wilk	Normality
Age	35.2	12.5	18	65	32	28	38	35	0.15	2.1	0.98	Normal
Gender	1.2	0.4	1	2	1	1	1	1	0.05	0.2	0.95	Normal
Marital Status	2.1	0.8	1	3	2	1	3	2	0.12	1.8	0.97	Normal
Education	15.8	2.5	10	20	16	15	17	16	0.08	0.5	0.99	Normal
Income	1200	300	500	2000	1100	900	1300	1000	0.18	2.5	0.96	Normal
Occupation	1.5	0.5	1	3	2	1	3	2	0.05	0.2	0.95	Normal
Health Status	2.5	0.5	1	3	2	2	2	2	0.02	0.1	0.99	Normal
Stress Level	3.2	1.0	1	5	3	2	4	3	0.15	2.1	0.98	Normal
Life Satisfaction	4.5	0.8	3	5	4	4	4	4	0.02	0.1	0.99	Normal
Work-Life Balance	3.8	0.9	2	5	4	3	4	4	0.05	0.2	0.95	Normal
Family Support	4.2	0.7	3	5	4	4	4	4	0.02	0.1	0.99	Normal
Community Involvement	2.8	0.6	1	4	3	2	3	3	0.08	0.5	0.99	Normal
Personal Growth	3.5	0.9	2	5	3	3	4	3	0.12	1.8	0.97	Normal
Overall Well-being	4.0	0.8	3	5	4	4	4	4	0.02	0.1	0.99	Normal

heptalene|heptalen root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,5a, Ring, Ring2, c,6, c,7, c,8, c,9, c,10, c,10a, Ring, Ring1, Ring, Ring2
 asindacene|asindacen root root
 c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,5, c,5a, Ring, Ring3, c,6, c,7, c,8, c,8a, Ring, Ring3, c,8b, Ring, Ring2, Ring, Ring1
 sindacene|sindacen root root
 c,1, Ring, Ring1, c,2, c,3, c,3a, Ring, Ring2, c,4, c,4a, Ring, Ring3, c,5, c,6, c,7, c,7a, Ring, Ring3, c,8, c,8a, Ring, Ring2, Ring, Ring1
 octalene|octalen root root
 c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,6, c,6a, Ring, Ring2, c,7, c,8, c,9, c,10, c,11, c,12, c,12a, Ring, Ring1, Ring, Ring2
 mevalon root root C,1, C,2, C,3, (, x, C,4, C,5, O, x,) (, x, O, x,) , x, C, x
 lact|lactyl root root C,1, C,2 |alpha|a, (, x, O, x,) , x, C,3 |b|beta
 24d root root
 O,1@x, C, x, (=, x, O, x,) , x, C, a|alpha, O, x, c,1, Ring, Ring1, c,2, (, x, Cl, x,) , x, c,3, c,4, (, x, Cl, x,) , x, c,5, c,6, Ring, Ring1
 245t root root
 O,1@x, C, x, (=, x, O, x,) , x, C, a|alpha, O, x, c,1, Ring, Ring1, c,2, (, x, Cl, x,) , x, c,3, c,4, (, x, Cl, x,) , x, c,5, (, x, Cl, x,) , x, c,6, Ring, Ring1
 dnp|24dnp root root c,4@1, Ring, Ring1, c, x, ([N+] (=O) [O-]), x, c,3|m|meta, c, x, ([N+] (=O) [O-]), x, c,5, c,6, Ring, Ring1
 morphol root root C,2, Ring, Ring1, C,3, N,4, C,5, C,6, O,1, Ring, Ring1
 morpholino root root O,1, Ring, Ring1, C,2, C,3, N,4@4, C,5, C,6, Ring, Ring1
 semicarbazide|semicarbazid root root N,1, N,2, C, x, (=, x, O,3,) , x, N,4
 semicarbazido root root N,4@1, N,2, C, x, (=, x, O,3,) , x, N,4
 isosemicarbazide|isosemicarbazid root root N,1, N,2, C, x, (, x, O,3,) =, x, N,4
 isosemicarbazido root root N,4@1, N,2, C, x, (, x, O,3,) =, x, N,4
 semicarbazono root root N,8@1, N,2, C, x, (=, x, O,3,) , x, N,4
 carbaz root root C,1, N,2, N,3
 acetone|aceton root alkane C,1|a|alpha, C, x, (=O) , x, C,3 |w|omega
 acetylacetone root root C,1, C,2, (=, x, O, x,) , x, C,3, C,4, (=, x, O, x,) , x, C,5
 isobutyron|isobutyron root root CC(C)C(=O)C(C)C, x
 isovalerone|isovaleron root root CC(C)CC(=O)CC(C)C, x
 enanthone root alkane
 C,1, C,2 |a|alpha, C,3 |b|beta, C,4 |g|gamma, C,5 |d|delta, C,6 |e|epsilon, C,7, (=O) , x, C,8, C,9, C,10, C,11, C,12, C,13 |w|omega
 pelargone root alkane
 C,1, C,2 |a|alpha, C,3 |b|beta, C,4 |g|gamma, C,5 |d|delta, C,6 |e|epsilon, C,7, C,8, C,9, (=O) , x, C,10, C,11, C,12, C,13, C,14, C,15, C,16, C,17, C,18 |w|omega
 laurone root alkane
 C,1|a|alpha, C,2, C,3, C,4, C,5, C,6, C,7, C,8, C,9, C,10, C,11, C, x, (=O) , x, C,13, C,14, C,15, C,16, C,17, C,18, C,19, C,20, C,21, C,22, C,23 |w|omega
 myristone root alkane
 C,1|a|alpha, C,2, C,3, C,4, C,5, C,6, C,7, C,8, C,9, C,10, C,11, C,12, C,13, C, x, (=O) , x, C,15, C,16, C,17, C,18, C,19, C,20, C,21, C,22, C,23, C,24, C,25, C,26, C,27 |w|omega
 palmitone root alkane
 C,1|a|alpha, C,2, C,3, C,4, C,5, C,6, C,7, C,8, C,9, C,10, C,11, C,12, C,13, C,14, C,15, C, x, (=O) , x, C,17, C,18, C,19, C,20, C,21, C,22, C,23, C,24, C,25, C,26, C,27, C,28, C,29, C,30, C,31 |w|omega
 stearone root alkane
 C,1|a|alpha, C,2, C,3, C,4, C,5, C,6, C,7, C,8, C,9, C,10, C,11, C,12, C,13, C,14, C,15, C,16, C,17, C, x, (=O) , x, C,19, C,20, C,21, C,22, C,23, C,24, C,25, C,26, C,27, C,28, C,29, C,30, C,31, C,32, C,33, C,34, C,35 |w|omega
 silatrane|silatran root root
 [Si],1, Ring, Ring1, Ring, Ring2, O,2, C,3, C,4, N,5, (, x, C,6, C,7, O,8, Ring, Ring1,) , x, C,11, C,10, O,9, Ring, Ring2

[illegible]

```

isocoumarin|isocoumarin root root
C,1, Ring, Ring1, (=, x, O, x, ), x, o, 2, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, c, 7, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
coumaran root root
O,1, Ring, Ring1, C, 2, C, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring1, Ring, Ring2
coumarone|coumaron root root
o,1, Ring, Ring1, c, 2, c, 3, c, 3a, Ring, Ring2, c, 4, c, 5, c, 6, c, 7, c, 7a, Ring, Ring1, Ring, Ring2
ayapin root root
o,1, Ring, Ring1, c, 2, (=, x, O, x, ), x, c, 3, c, 4, c, 4a, Ring, Ring2, c, 5, c, 6, (, x, COC, x, Ring, Ring3, ), x, c, 7, Ring, Ring3, c, 8, c, 8a, Ring, Ring1, Ring, Ring2
benzhydr root root
C,a|alpha, (, x, c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, Ring, Ring1, ), x, c, 1', Ring, Ring2, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring2
benzoguanamine|benzoguanamin root root
c,1, (, x, Ring, Ring1, n, 2, c, 3, (, x, N, x, ), x, n, 4, c, 5, (, x, N, x, ), x, n, 6, Ring, Ring1, ), x, c, 1', Ring, Ring2, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring2
trit root root
C,a|alpha, Ring, Ring1, Ring, Ring2, Ring, Ring3, ., x, c, 4, Ring, Ring4, Ring, Ring5, ., x, c, 4', Ring, Ring6, Ring, Ring7, ., x, c, 4'', Ring, Ring8, Ring, Ring9, ., x, c, 3, Ring, Ring4, c, 2, c, 1, Ring, Ring1, c, 6, c, 5, Ring, Ring5, ., x, c, 3', Ring, Ring6, c, 2', c, 1', Ring, Ring2, c, 6', c, 5', Ring, Ring7, ., x, c, 3'', Ring, Ring8, c, 2'', c, 1'', Ring, Ring3, c, 6'', c, 5'', Ring, Ring9
ureth root root N,n,C,x, (=, x, O, x, ), x, O, x, C, x, C, x
chalcone|chalcon root root
C,a|alpha, (, x, C, x, (=, x, O, x, ), x, c, 1', Ring, Ring1, c, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring1, ), x, =, x, C, b|beta, c, 1, Ring, Ring2, c, 2, c, 3, c, 4, c, 5, c, 6, Ring, Ring2
deoxybenzoin root root
C,a|alpha, (, x, C, x, (=O), x, c, 1, Ring, Ring1, c, 2, c, 3, c, 4, c, 5, c, 6, Ring, Ring1, ), x, c, 1', Ring, Ring2, =, x, C, 2', c, 3', c, 4', c, 5', c, 6', Ring, Ring2
thiurammonosulfide|thiurammonosulfid root root
N,n,C,x, (=, x, S, x, ), x, S, x, C, x, (=, x, S, x, ), x, N, n'
thiuramdisulfide|thiuramdisulfid root root
N,n,C,x, (=, x, S, x, ), x, SS, x, C, x, (=, x, S, x, ), x, N, n'
thiuramtrisulfide|thiuramtrisulfid root root
N,n,C,x, (=, x, S, x, ), x, SSS, x, C, x, (=, x, S, x, ), x, N, n'
thiuramtetrasulfide|thiuramtetrasulfid root root
N,n,C,x, (=, x, S, x, ), x, SSSS, x, C, x, (=, x, S, x, ), x, N, n'
mercuran root root S=C(SSC(N(C)C)=S)N(C)C,x
diacetamide|diacetamid root root
N,n, (, x, C, x, (, x, =, x, O, x, ), x, C, x, ), x, C, x, (, x, =, x, O, x, ), x, C, x
triacetamide|triacetamid root root
N,x, (, x, C, x, (, x, =, x, O, x, ), x, C, x, ), x, (, x, C, x, (, x, =, x, O, x, ), x, C, x, ), x, C, x, (, x, =, x, O, x, ), x, C, x
dibenzamide|dibenzamid root root
N,n, (, x, C, x, (, x, =, x, O, x, ), x, c, x, Ring, Ring1, ccccc, x, Ring, Ring1, ), x, C, x, (, x, =, x, O, x, ), x, c, x, Ring, Ring2, ccccc, x, Ring, Ring2
tribenzamide|tribenzamid root root
N,x, (, x, C, x, (, x, =, x, O, x, ), x, c, x, Ring, Ring1, ccccc, x, Ring, Ring1, ), x, (, x, C, x, (, x, =, x, O, x, ), x, c, x, Ring, Ring2, ccccc, x, Ring, Ring2, ), x, C, x, (, x, =, x, O, x, ), x, c, x, Ring, Ring3, =, x, ccccc, x, Ring, Ring3
fulvene|fulven root root
C,6, =, x, C, 5, Ring, Ring1, C, 1, =, x, C, 2, C, 3, =, x, C, 4, Ring, Ring1
stilbene|stilben root root
C,b|beta|a'|alpha', (=, x, C, a|alpha, c, 1, Ring, Ring1, c, 2|o|ortho, c, 3|m|meta, c, 4|p|para

```

ra,c,5,c,6, Ring, Ring1,), x,c,1', Ring, Ring2, c,2' |o' |ortho', c,3' |m' |meta', c,4' |p' |p
 ara', c,5', c,6', Ring, Ring2
 stilbestrol|stilboestrol root root
 C,b|beta, (=, x,C,a|alpha, c,1, Ring, Ring1, c,2, c,3, c,4, (O), x,c,5,c,6, Ring, Ring1,), x,
 c,1', Ring, Ring2, c,2', c,3', c,4', (O), x,c,5', c,6', Ring, Ring2
 hexestrol root root
 C,b|beta, (CC) (, x,C,a|alpha, (CC), x,c,1, Ring, Ring1, c,2, c,3, c,4, (O), x,c,5,c,6, Ring,
 Ring1,), x,c,1', Ring, Ring2, c,2', c,3', c,4', (O), x,c,5', c,6', Ring, Ring2
 benzil root root
 C(=O), x, (, x,C(=O), x,c,1, Ring, Ring1, c,2, c,3, c,4, c,5, c,6, Ring, Ring1,), x,c,1', Ring,
 Ring2, c,2', c,3', c,4', c,5', c,6', Ring, Ring2
 antipyr|antipylene|phenazone root root
 C,4, Ring, Ring1, C,5, (=O), x,N,1, (, x,N,2, (, x,C,x,), x,C,3, (, x,C,x,), x,=, x, Ring, Ring1
 ,), x,c,1', Ring, Ring2, c,2', c,3', c,4', c,5', c,6', Ring, Ring2
 glycid root root C,1,C,2|b|beta, Ring, Ring1, C,3,O,x, Ring, Ring1
 ketene|keten root root C=C=O,1
 diketene|diketen root root C=C1CC(=O)O1,x
 adamant root root
 C,1, Ring, Ring1, Ring, Ring2, C,2,C,3, Ring, Ring3, C,4,C,5, (, x,C,6,C,7, (, x,C,8, Ring, Ri
 ng1,), x,C,10, Ring, Ring3,), x,C,9, Ring, Ring2
 noradamant root root
 C,1, Ring, Ring1, Ring, Ring2, C,2,C,3, Ring, Ring3, C,4,C,5, (, x,C,6,C,7, (, x,C,8, Ring, Ri
 ng1,), x, Ring, Ring3,), x,C,9, Ring, Ring2
 hexamethylenetetramine|hexamethylenetetramin root root
 N,1, Ring, Ring1, Ring, Ring2, C,2,N,3, Ring, Ring3, C,4,N,5, (, x,C,6,N,7, (, x,C,8, Ring, Ri
 ng1,), x,C,10, Ring, Ring3,), x,C,9, Ring, Ring2
 pentamethylenetetramine|pentamethylenetetramin root root N12CNCN(CNC1)C2,x
 fulvalene|fulvalen root root
 c,2, Ring, Ring1, (, x,c,3,c,4,c,5,c,1, Ring, Ring1,)=, x,c,2', Ring, Ring2, c,3', c,4', =, x
 ,c,5', c,1', Ring, Ring2
 tetrathiafulvalene|tetrathiafulvalen root root
 C,2, Ring, Ring1, (, x,S,3,C,4, =, x,C,5,S,1, Ring, Ring1,)=, x,C,2', Ring, Ring2, S,3', C,4'
 , =, x,C,5', S,1', Ring, Ring2
 tetraselenafulvalene|tetrathiafulvalen root root
 C,2, Ring, Ring1, (, x, [Se], 3,C,4, =, x,C,5, [Se], 1, Ring, Ring1,)=, x,C,2', Ring, Ring2, [Se
], 3', C,4', =, x,C,5', [Se], 1', Ring, Ring2
 labd root natural
 C,1, Ring, Ring1, C,2,C,3, [C@@], 4, (, x,C,18,), x, (, x,C,19,), x, [C@@], 5, ([H]), x, Ring, Ri
 ng2, C,6,C,7, [C@], 8|a-r, (, x,C,17,), x, [C@@], 9|a-
 b, (, x, [C@], 10, Ring, Ring2, Ring, Ring1, C,20,), x,C,11|a-
 t, C,12, [C@], 13, (, x,C,16,), x,C,14,C,15
 ambros root natural C,2, Ring, Ring1, C,3,C,4, [C@@], 5|a-
 b, Ring, Ring2, (, x,C,15,), x,C,6|a-
 r, [C@], 7, (, x,C,11, (, x,C,12,), x,C,13,), x,C,8,C,9, [C@], 10, (, x,C,14,), x, [C@@], 1|a-
 t, ([H]), x, Ring, Ring2, Ring, Ring1
 cedr root natural [C@@], 2, Ring, Ring1, (, x,C,12,), x,C,3,C,4, [C@], 5|a-
 b, ([H]), x, Ring, Ring2, [C@@], 6|a-
 r, (, x,C,13,), x, (, x,C,14,), x, [C@], 7, (, x,C,11, Ring, Ring3,), x, [C@], 8, (, x,C,15,), x,C
 ,9,C,10, [C@@], 1|a-t, Ring, Ring1, Ring, Ring2, Ring, Ring3
 cedrol root natural OC1(C)C3CC2(C(C3(C)C)CCC2C)CC1,x
 apotrichothec root natural
 O,1, Ring, Ring1, [C@], 12, Ring, Ring2, (, x,C,13,), x,C,2,C,3,C,4, [C@@], 5|a-
 r, (, x,C,14,), x, Ring, Ring2, [C@], 6|a-
 b, (, x,C,15,), x, Ring, Ring3, C,7,C,8,C,9, (, x,C,16,), x,C,10, [C@], 11|a-
 t, ([H]), x, Ring, Ring3, Ring, Ring1

[illegible]

[illegible]

[illegible]

[illegible]

cc9),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergocryptine|ergocryptin|ergocriptine|ergocriptin|alphaergocryptine|alphaergocryptin|alphaergocriptine|alphaergocriptin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 betaergocryptine|betaergocryptin|betaergocriptine|betaergocriptin|bergocryptine|bergocryptin|bergocriptine|bergocriptin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergocryptinine|ergocryptinin|ergocriptinine|ergocriptinin|alphaergocryptinine|alphaergocryptinin|alphaergocriptinine|alphaergocriptinin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 betaergocryptinine|betaergocryptinin|betaergocriptinine|betaergocriptinin|bergocryptinine|bergocryptinin|bergocriptinine|bergocriptinin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(C(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergosine|ergosin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ergotamine|ergotamin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(Cc9cccc9),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 bromocryptine|bromocryptin|bromocriptine|bromocriptin root natural c,a-t,Ring,Ring1,c,a-b,Ring,Ring2,c,a-
 1,Ring,Ring3,c,x,c,x,c,x,c,x,(x,N,1,c,2,(Br),x,Ring,Ring4),x,c,x,Ring,Ring3,c,x,Ring,Ring4,C,x,[C@],8,([H]),x,Ring,Ring2,N,x,(C),x,C,x,[C@@H],x,Ring,Ring1,C,18,(=O),x,N,x,[C@],2',(C(C)C),x,Ring,Ring5,C,3',(=O),x,N,4',Ring,Ring6,[C@@H],5',(CC(C)C),x,C,6',(=O),x,N,7',Ring,Ring7,C,8',C,9',C,10',[C@],11',([H]),x,Ring,Ring7,[C@@],12',(O),x,Ring,Ring6,O,1',Ring,Ring5
 ecgonidine|ecgonidin root root
 [C@@],x,([H]),x,Ring,Ring1,Ring,Ring2,C,x,c,x,c,x,(x,C,x,(=O),x,O,1@x),x,[C@],x,([H]),x,(x,N,x,(C),x,Ring,Ring1),x,C,x,C,x,Ring,Ring2

ecgonine|ecgonin root root
 [C@@],x,([H]),x, Ring, Ring1, Ring, Ring2, C, x, [C@H], x, (O), x, [C@H], x, (, x, C, x, (=O), x, O
 , 1@x,), x, [C@], x, ([H]), x, (, x, N, x, (C), x, Ring, Ring1,), x, C, x, C, x, Ring, Ring2
 methylviologen root root
 c, 1, Ring, Ring1, (, x, c, 2, c, 3, [n+], 4, (C), x, c, 5, c, 6, Ring, Ring1,), x, c, 1', Ring, Ring2, c
 , 2', c, 3', [n+], 4', (C), x, c, 5', c, 6', Ring, Ring2
 ethylviologen root root
 c, 1, Ring, Ring1, (, x, c, 2, c, 3, [n+], 4, (CC), x, c, 5, c, 6, Ring, Ring1,), x, c, 1', Ring, Ring2,
 c, 2', c, 3', [n+], 4', (CC), x, c, 5', c, 6', Ring, Ring2
 benzylviologen root root
 c, 1, Ring, Ring1, (, x, c, 2, c, 3, [n+], 4, (Cc3ccccc3), x, c, 5, c, 6, Ring, Ring1,), x, c, 1', Ring
 , Ring2, c, 2', c, 3', [n+], 4', (Cc4ccccc4), x, c, 5', c, 6', Ring, Ring2
 pheneturide root root O=C(N)NC(C(C)C1=CC=CC=C1)=O, x
 lactide|dilactide root root CC(OC1=O)C(OC1C)=O, x
 gallion root root OC(C(C1)=CC([N+])([O-]
))=O)=C3)=C3N=NC1=C(S(=O)(O)=O)C=C(C(=S(=O)(O)=O)C=C2N)C2=C1O, x
 clobfibr root root CC(C)(OC1=CC=C(C=C1)C1)C, x
 paraben root root O, 1@x, C(C1=CC=C(O)C=C1)=O, x
 edetate|versenate|edta root root
 O, 1@x, C(CN(CC(, x, O, 1@x,)=O)CCN(CC(, x, O, 1@x,)=O)CC(, x, O, 1@x,)=O)=O, x
 fusar root root CC1=CC=C(CCCC)C=N1, x
 lironion root root COC1=CC=C(OC2=CC=C(C=C2)NC(N(C)C)=O)C=C1, x
 thionalide root root O=C(CS)NC2=CC1=CC=CC=C1C=C2, x
 tolperisone root root CC(C(C2=CC=C(C)C=C2)=O)CN1CCCCC1, x
 valethamate root root CCC(C(C(OC[N+](CC)(CC)C)=O)C1=CC=CC=C1)C, x
 secbutabarbital|butalan root root O=C(N1)NC(C(C(C)CC)(CC)C1=O)=O, x
 furalan root root O=C(N2)N(CC2=O)N=CC1=CC=C([N+])([O-])=O)O1, x
 boc|tboc root nprotect C, 4@x, (=O)OC(C)(C)C, x
 z-nprot root nprotect C, 4@x, (=O)OCc1cccc1, x
 msoc root nprotect C, 4@x, (=O)OCCS(=O)(=O)C, x
 cbz root nprotect
 C, 4@x, (=O)OC, x, C, 1, Ring, Ring1, =, x, C, 2, C, 3, =, x, C, 4, C, 5, =, x, C, 6, Ring, Ring1
 fmoc root nprotect C, 4@x, (=O)OCC1C2=CC=CC=C(C3=CC=CC=C13)2, x
 dansyl root nprotect S, 4@x, (C2=CC=CC1=C(N(C)C)C=CC=C12)(=O)=O, x
 dabsyl root nprotect S, 4@x, (c1ccc(N=Nc2ccc(N(C)C)cc2)cc1)(=O)=O, x
 bansyl root nprotect S, 4@x, (C2=CC=CC1=C(N(CCCC)CCCC)C=CC=C12)(=O)=O, x
 nps root nprotect S, 4@x, c1c([N+](=O)[O-])cccc1, x
 tfa root nprotect C, 4@x, (=O)C(F)(F)F, x
 acm root nprotect C, 4@x, NC(=O)C, x
 phacm root nprotect C, 4@x, NC(=O)Cc1cccc1, x
 creatine root root CN(C(N)=N)CC(O)=O, x
 panthenol root root CC(CO)(C(C(NCCCCO)=O)O)C, x
 alanate root root [AlH4-], x
 cyanamide root root NC#N, x
 eprolin root root CC1=C2C(OC(CCCC(C)CCCC(C)CCCC(C)C)(C)CC2)=C(C)C(C)=C1O, x
 eserine|physostigmine root root O=C(NC)OC1=CC=C(N(C)C3C2(C)CCN3C)C2=C1, x
 prolan root root CC([N+])([O-])=O)C(C2=CC=C(C1)C=C2)C1=CC=C(C1)C=C1, x
 tropanserine root root CN1C2CCC1CC(OC(C3=CC(C)=CC(C)=C3)=O)C2, x
 butanserine root root FC1=CC=C(C(C4CCN(CC4)CCCCN3C(NC2=CC=CC=C2C3=O)=O)=O)C=C1, x
 amiprol|domalium|kiatrium|levium|relanium|tensium|umbrium|velium|valium root
 root O=C1CN=C(C3=CC=CC=C3)C2=C(C=CC(C1)=C2)N1C, x
 prolate root root S=P(OC)(OC)SCN1C(C(C=CC=C2)=C2C1=O)=O, x
 adaprolol root root CC(NCC(COC4=CC=C(C=C4)CC(OCCC23CC1CC(C3)CC(C2)C1)=O)O)C, x
 agmatine root root NC(NCCCCN)=N, x
 algolysin root root CCC(C(C1=CC=CC=C1)(C2=CC=CC=C2)CC(C)N(C)C)=O.[H]C1, x
 altanserine root root FC1=CC=C(C(C2CCN(CCN4C(NC3=CC=CC=C3C4=O)=S)CC2)=O)C=C1, x

[illegible]

[illegible]

ng,Ring1,) ,x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,
 Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,O,1',Ring,Ring3
 oxatricarbocyanine root root
 o,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
 ng,Ring1,) ,x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,13,C,14,=,x,C,2',Ring,Ring3,N,
 3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,O,1',Ring,Ring3
 thiacyanine root root
 s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
 ng,Ring1,) ,x,C,8,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c
 ,7a',Ring,Ring4,S,1',Ring,Ring3
 thiacarboxyanine root root
 s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
 ng,Ring1,) ,x,C,8,=,x,C,9,C,10,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4',c,5
 ',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
 thiadicarbocyanine root root
 s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
 ng,Ring1,) ,x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,
 Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
 thiatricarbocyanine root root
 s,1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring2,Ri
 ng,Ring1,) ,x,C,8,=,x,C,9,C,10,=,x,C,11,C,12,=,x,C,13,C,14,=,x,C,2',Ring,Ring3,N,
 3',c,3a',Ring,Ring4,c,4',c,5',c,6',c,7',c,7a',Ring,Ring4,S,1',Ring,Ring3
 selenacarboxyanine root root
 [se],1,Ring,Ring1,c,2,(,x,[n+],3,c,3a,Ring,Ring2,c,4,c,5,c,6,c,7,c,7a,Ring,Ring
 2,Ring,Ring1,) ,x,C,8,=,x,C,9,C,10,=,x,C,2',Ring,Ring3,N,3',c,3a',Ring,Ring4,c,4'
 ,c,5',c,6',c,7',c,7a',Ring,Ring4,[Se],1',Ring,Ring3
 hordenine root root CN(C)CCC1=CC=C(O)C=C1,x
 maltol root root O=C(C)C(=O)C(=O)C1=CC=C(C)C1,x
 coman root root Cc1=cc(=O)ccO1,x
 chrysoidine root root
 c,4|p|para,(,x,c,3|m|meta,c,2|o|ortho,Ring,Ring1,) ,x,c,5,c,6,c,1,Ring,Ring1,N=Nc
 2c(N)cc(N)cc2,x
 alphafuril root root O=C(C1=CC=CC1)C(C2=CC=CC2)=O,x
 anisil root root O=C(C1=CC=C(OC)C=C1)C(C2=CC=C(OC)C=C2)=O,x
 alphaphellandrene root root CC1=CCC(C(C)C)C=C1,x
 betaphellandrene root root CC(C(C=C1)CCC1=C)C,x
 scopolamine|scopolamin root root C[N+](=O)C1=CC(OC(C(CO)C3=CC=CC=C3)=O)C2,x
 pilocarpine|pilocarpin root root CC[C@H]1[C@@H](CC2=CN=CN2C)COC1=O,x
 guanethidine root root NC(NCCN1CCCCCCC1)=N,x
 lobeline root root CN1C(CC(C3=CC=CC=C3)O)CCCC1CC(C2=CC=CC=C2)=O,x
 mercaptur root root C[C@H](CS)NC(C)=O,x
 phenylmercaptur root root C[C@H](CSc1ccccc1)NC(C)=O,x
 alphasip|alip root root CCCCC1SSCC1,x
 perill|perilla root root CC1=CCC(C(C)=C)CC1,x
 biotin root root O,1@x,C(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
 biotinyl root root C,4@x,(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
 biotinamide|biotinamid root root
 N,x,C(CCCC[C@H]1[C@](NC2=O)([H])[C@](N2)([H])CS1)=O,x
 bisphenola root root
 O1.Oc,4,Ring,Ring2,c,5,c,6,c,1,(,x,c,2,c,3,Ring,Ring2,) ,x,C(C)(C),x,c,1',Ring,Ri
 ng3,c,2',c,3',c,4',Ring,Ring1,c,5',c,6',Ring,Ring3
 pantothen root root CCCNC(C(C(CO)(C)C)O)=O,x
 alloxan root root
 N,1,Ring,Ring1,C,2,(=O),x,N,3,C,4,(=O),x,C,5,(=O),x,C,6,(=O),x,Ring,Ring1
 croman root root Cc1occc(=O)c1,x

[illegible]

ng,Ring4,C,15,C,16,C,17,[C@@],13,Ring,Ring4,(,x,C,18,) ,x,C,12,C,11,C,9,Ring,Ring
3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
etioallochola|etioallochol root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,) ,x,C,4,[C@@],5,([H]),x,Ring,Ring2,C,6,C,7,C,8,Ring,R
ing3,C,14,Ring,Ring4,C,15,C,16,C,17,[C@@],13,Ring,Ring4,(,x,C,18,) ,x,C,12,C,11,C
,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
etien root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,) ,x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(C),x,[C@@],13,Ring,Ring4,(,x,C,18,) ,x,C,12,C,11,
C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
etian root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,) ,x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(C),x,[C@@],13,Ring,Ring4,(,x,C,18,) ,x,C,12,C,11,C,9,
Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
androstenediol root steroid
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,) ,x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,C,8,Ring
,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@H],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,) ,x
,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
androstenedione root steroid
C,3,(=O),x,(,x,C,2,C,1,Ring,Ring1,) ,x,C,4,=,x,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ri
ng3,C,14,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,18,) ,x,C,12,
C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
pregna|pregn root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,) ,x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,C,20,C,21,) ,x,[C@@],13,Ring,Ring4,(,x,C,18,) ,x,C,
12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
allopregna|allopregn root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,) ,x,C,4,[C@@],5,([H]),x,Ring,Ring2,C,6,C,7,C,8,Ring,R
ing3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,C,21,) ,x,[C@@],13,Ring,Ring4,(,x
,C,18,) ,x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
chola|chol root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,) ,x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@H],20,(,x,C,22,C,23,C,24,) ,x,C,21,) ,x,[C@@],1
3,Ring,Ring4,(,x,C,18,) ,x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring
2,C,19
cholesta|cholest|coprost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,) ,x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,Ri
ng,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,) ,x,C,2
7,) ,x,C,21,) ,x,[C@@],13,Ring,Ring4,(,x,C,18,) ,x,C,12,C,11,C,9,Ring,Ring3,[C@@],1
0,Ring,Ring1,Ring,Ring2,C,19
lanosta|lanost root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,) ,x,[C@],4,(,x,C,28,) (,x,C,29,) ,x,C,5,Ring,Ring2,C,6,
C,7,C,8,Ring,Ring3,[C@],14,Ring,Ring4,(,x,C,30,) ,x,C,15,C,16,[C@],17,(,x,[C@@],2
0,(,x,C,22,C,23,C,24,C,25,(,x,C,26,) ,x,C,27,) ,x,C,21,) ,x,[C@@],13,Ring,Ring4,(,x
,C,18,) ,x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
dammara|dammar root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,) ,x,[C@],4,(,x,C,28,) (,x,C,29,) ,x,C,5,Ring,Ring2,C,6,
C,7,C,8,Ring,Ring3,[C@@],14,Ring,Ring4,(,x,C,30,) ,x,C,15,C,16,[C@],17,(,x,[C@@],
20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,) ,x,C,27,) ,x,C,21,) ,x,[C@@],13,Ring,Ring4,C,
12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
urs root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,) ,x,C,4,(,x,C,x,) (,x,C,x,) ,x,C,5,Ring,Ring2,C,6,C,7,[
C@],8,(C),x,Ring,Ring3,[C@],14,Ring,Ring4,(C),27,C,x,C,x,[C@@],x,Ring,Ring5,(C),
28,C,22,C,21,[C@@H],20,(,x,C,30,) ,x,[C@H],19,(,x,C,29,) ,x,[C@@],18,([H]),x,Ring,
Ring5,[C@@],13,Ring,Ring4,(,x,[H],x,) ,x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,R
ing1,Ring,Ring2,C,x

[illegible]

,20,(,x,C,22,C,23,C,24,C,25,(,x,C,26,) ,x,C,27,) ,x,C,21,) ,x,[C@@],13, Ring, Ring4, (,x,C,18,) ,x,C,12,C,11,C,9, Ring, Ring3, [C@@],10, Ring, Ring1, Ring, Ring2, C,19
ergosta|ergost root steroid
C,3,(,x,C,2,C,1, Ring, Ring1,) ,x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ri
ng, Ring4, C,15,C,16, [C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(C) ,x,C,25,(,x,C,
26,) ,x,C,27,) ,x,C,21,) ,x,[C@@],13, Ring, Ring4, (,x,C,18,) ,x,C,12,C,11,C,9, Ring, Rin
g3, [C@@],10, Ring, Ring1, Ring, Ring2, C,19
campesta|campest root steroid
C,3,(,x,C,2,C,1, Ring, Ring1,) ,x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ri
ng, Ring4, C,15,C,16, [C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(C) ,x,C,25,(,x,C,
26,) ,x,C,27,) ,x,C,21,) ,x,[C@@],13, Ring, Ring4, (,x,C,18,) ,x,C,12,C,11,C,9, Ring, Ri
ng3, [C@@],10, Ring, Ring1, Ring, Ring2, C,19
poriferasta|poriferast root steroid
C,3,(,x,C,2,C,1, Ring, Ring1,) ,x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ri
ng, Ring4, C,15,C,16, [C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(CC) ,x,C,25,(,x,C,
26,) ,x,C,27,) ,x,C,21,) ,x,[C@@],13, Ring, Ring4, (,x,C,18,) ,x,C,12,C,11,C,9, Ring, Ri
ng3, [C@@],10, Ring, Ring1, Ring, Ring2, C,19
stigmasta|stigmast root steroid
C,3,(,x,C,2,C,1, Ring, Ring1,) ,x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ri
ng, Ring4, C,15,C,16, [C@],17,(,x,[C@@],20,(,x,C,22,C,23,[C@H],24,(,x,C,28,C,29,) ,
x,C,25,(,x,C,26,) ,x,C,27,) ,x,C,21,) ,x,[C@@],13, Ring, Ring4, (,x,C,18,) ,x,C,12,C,11
,C,9, Ring, Ring3, [C@@],10, Ring, Ring1, Ring, Ring2, C,19
pregnenolone root steroid
C,1, Ring, Ring1, C,2,C,3, (O) ,x,C,4,c,5, Ring, Ring2, c,6,C,7,C,8, Ring, Ring3, C,14, Ring
, Ring4, C,15,C,16, [C@],17,(,x,C,20,(=O) ,x,C,21,) ,x,[C@@],13, Ring, Ring4, (,x,C,18,) ,
x,C,12,C,11,C,9, Ring, Ring3, [C@@],10, Ring, Ring1, Ring, Ring2, C,19
prednisolone|prednisolon root steroid
C,1, Ring, Ring1, =,x,C,2,C,3, (=O) ,x,C,4, =,x,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3,
C,14, Ring, Ring4, C,15,C,16, [C@@],17,(,x,C,20,(=O) ,x,C,21,O,x,) ,x,(,x,O,x,) ,x,[C@@
],13, Ring, Ring4, (,x,C,18,) ,x,C,12,C,11,(,x,O,x,) ,x,C,9, Ring, Ring3, [C@@],10, Ring,
Ring1, Ring, Ring2, C,19
progesterone|progesteron root steroid
C,1, Ring, Ring1, C,2,C,3, (=O) ,x,c,4,c,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Rin
g, Ring4, C,15,C,16, [C@],17,(,x,C,20,(=O) ,x,C,21,) ,x,[C@@],13, Ring, Ring4, (,x,C,18,
) ,x,C,12,C,11,C,9, Ring, Ring3, [C@@],10, Ring, Ring1, Ring, Ring2, C,19
tetrahydroprogesterone|tetrahydroprogesteron root steroid
C,1, Ring, Ring1, C,2,C,3, (O) ,x,c,4,c,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ring
, Ring4, C,15,C,16, [C@],17,(,x,C,20,(O) ,x,C,21,) ,x,[C@@],13, Ring, Ring4, (,x,C,18,) ,
x,C,12,C,11,C,9, Ring, Ring3, [C@@],10, Ring, Ring1, Ring, Ring2, C,19
hydrocortisone|hydrocortison root steroid
C,1, Ring, Ring1, C,2,C,3, (=O) ,x,C,4, =,x,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14
, Ring, Ring4, C,15,C,16, [C@@],17,(,x,C,20,(=O) ,x,C,21,O,x,) ,x,(,x,O,x,) ,x,[C@@],13
, Ring, Ring4, (,x,C,18,) ,x,C,12, [C@H],11, (O) ,x,C,9, Ring, Ring3, [C@@],10, Ring, Ring1
, Ring, Ring2, C,19
dihydrocortisone|dihydrocortison root steroid
C,1, Ring, Ring1, C,2,C,3, (=O) ,x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Rin
g, Ring4, C,15,C,16, [C@@],17,(,x,C,20,(=O) ,x,C,21,O,x,) ,x,(,x,O,x,) ,x,[C@@],13, Rin
g, Ring4, (,x,C,18,) ,x,C,12, [C@H],11, (=O) ,x,C,9, Ring, Ring3, [C@@],10, Ring, Ring1, Ri
ng, Ring2, C,19
tetrahydrocortisone|tetrahydrocortison root steroid
C,1, Ring, Ring1, C,2, [C@H],3, (O) ,x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14
, Ring, Ring4, C,15,C,16, [C@@],17,(,x,C,20,(=O) ,x,C,21,O,x,) ,x,(,x,O,x,) ,x,[C@@],13
, Ring, Ring4, (,x,C,18,) ,x,C,12, [C@H],11, (O) ,x,C,9, Ring, Ring3, [C@@],10, Ring, Ring1
, Ring, Ring2, C,19
cortisone|cortison root steroid
C,1, Ring, Ring1, C,2,C,3, (=O) ,x,C,4, =,x,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14
, Ring, Ring4, C,15,C,16, [C@@],17,(,x,C,20,(=O) ,x,C,21,O,x,) ,x,(,x,O,x,) ,x,[C@@],13

```
,Ring,Ring4,(,x,C,18,),x,C,12,[C@H],11,(=O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring
1,Ring,Ring2,C,19
androsterone root steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9
,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
isoandrosterone root steroid
C,1,Ring,Ring1,C,2,[C@H],3,(O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14,
Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,
Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
aldosterone root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,)(=O),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,C,21,O,x,),x,[C@@],13,Ring,Ring4,(,x,C,1
8,=O,x,),x,C,12,[C@H],11,(O),x,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,1
9
pregnanolone root steroid
C,3,(O)(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,14
,Ring,Ring4,C,15,C,16,[C@],17,(,x,C,20,(=O),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C
,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
testosteron|testosterone root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,)(=O),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,
C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
dihydrotestosteron|dihydrotestosterone root steroid
C,3,(,x,C,2,C,1,Ring,Ring1,)(=O),x,C,4,C,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C,1
4,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,
C,9,Ring,Ring3,[C@@],10,Ring,Ring1,Ring,Ring2,C,19
oestradiol|estradiol|betaoestradiol|betaestradiol root steroid
c,3,(O),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
,14,Ring,Ring4,C,15,C,16,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11
,C,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
oestriol|estriol root steroid
c,3,(O),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
,14,Ring,Ring4,C,15,[C@@],16,(O),x,[C@],17,(O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x
,C,12,C,11,C,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
oestrone|estrone root steroid
c,3,(O),x,(,x,c,2,c,1,Ring,Ring1,),x,c,4,c,5,Ring,Ring2,C,6,C,7,C,8,Ring,Ring3,C
,14,Ring,Ring4,C,15,C,16,C,17,(=O),x,[C@@],13,Ring,Ring4,(,x,C,x,),x,C,12,C,11,C
,9,Ring,Ring3,c,10,Ring,Ring1,Ring,Ring2
brassinolid|brassinolide root steroid
[C@@H],3,(O),x,(,x,[C@H],2,(O),x,C,1,Ring,Ring1,),x,C,4,[C@],5,Ring,Ring2,([H]),
x,C,6,(=O)O,x,C,7,C,8,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,
(,x,[C@H],22,(O),x,[C@H],23,(O),x,[C@@H],24,(C),x,C,25,(,x,C,26,),x,C,27,),x,C,2
1,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C,9,Ring,Ring3,[C@@],10,Ring,Ri
ng1,Ring,Ring2,C,19
caldiol root root
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8,
Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C,2
5,(,x,C,26,)(O),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11,C
,9,Ring,Ring3,.,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
calciol|cholecalciferol|vitamind3 root root
[C@H],3,(O),x,(,x,C,2,C,1,Ring,Ring1,),x,C,4,C,5,Ring,Ring2,=,x,C,6,C,7,=,x,C,8|
a-
r,Ring,Ring3,C,14,Ring,Ring4,C,15,C,16,[C@],17,(,x,[C@@],20,(,x,C,22,C,23,C,24,C
,25,(,x,C,26,),x,C,27,),x,C,21,),x,[C@@],13,Ring,Ring4,(,x,C,18,),x,C,12,C,11|a-
t,C,9|a-b,Ring,Ring3,.,x,C,10,Ring,Ring1,Ring,Ring2,=,x,C,19
```

[illegible]

corticosterone root steroid

cortisol root steroid

ecdysone root steroid

ercalciol|ergocalciferol root root

ergosterol root steroid

lumisterol root steroid

cardanolide root steroid

card2022enolide|2022cardenolide root steroid

digitoxigenin root steroid

bufanolide root steroid

bufadienolide root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,), x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ring, Ring4, C,15,C,16, [C@], 17, (,x, [C@@], 20, Ring, Ring5, =, x,C,21,O,x,C,24, (=O), x,C,23, =, x,C,22, Ring, Ring5,), x, [C@@], 13, Ring, Ring4, (,x,C,18,), x,C,12,C,11,C,9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C,19

cev root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,), x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, [C@@], 14, ([H]), x, Ring, Ring4, C,15,C,16, [C@@], 17, ([H]), x, Ring, Ring5, [C@@H], 20, (C), x, [C@@], x, ([H]), x, Ring, Ring6, C,x,C,x, [C@H], x, (C), x,C,x,N,x, Ring, Ring6, C,x, [C@], x, ([H]), x, Ring, Ring5, [C@@], 12, ([H]), x, Ring, Ring4, C,11,C,9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C,19

solidan root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,), x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ring, Ring4, C,15,C,16, Ring, Ring5, [C@], 17, ([H]), (,x, [C@], 20, (,x,C,21,), x, [C@], 22, ([H]), x, Ring, Ring6, C,23,C,24, [C@H], 25, (,x,C,27,), x,C,26,N,28, Ring, Ring6, Ring, Ring5,), x, [C@@], 13, Ring, Ring4, (,x,C,18,), x,C,12,C,11,C,9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C,19

spirost root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,), x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ring, Ring4, C,15, [C@], 16, ([H]), (,x,O,x, Ring, Ring5,), x, [C@], 17, ([H]), (,x, [C@@], 20, (,x, [C@@], 22, Ring, Ring5, (,x,O,x, Ring, Ring6,), x,C,23,C,24,C,25, (,x,C,26, Ring, Ring6,), x,C,27,), x,C,21,), x, [C@@], 13, Ring, Ring4, (,x,C,18,), x,C,12,C,11,C,9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C,19

spirosol root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,), x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ring, Ring4, C,15, [C@], 16, ([H]), (,x,O,x, Ring, Ring5,), x, [C@], 17, ([H]), (,x, [C@], 20, (,x,C,22, Ring, Ring5, (,x,N,x, Ring, Ring6,), x,C,23,C,24,C,25, (,x,C,26, Ring, Ring6,), x,C,27,), x,C,21,), x, [C@@], 13, Ring, Ring4, (,x,C,18,), x,C,12,C,11,C,9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C,19

tomatid root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,), x,C,4, [C@@H], 5, ([H]), x, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ring, Ring4, C,15, [C@], 16, ([H]), (,x,O,x, Ring, Ring5,), x, [C@], 17, ([H]), (,x, [C@], 20, (,x, [C@], 22, Ring, Ring5, (,x,N,x, Ring, Ring6,), x,C,23,C,24, [C@@H], 25, (,x,C,26, Ring, Ring6,), x,C,27,), x,C,21,), x, [C@@], 13, Ring, Ring4, (,x,C,18,), x,C,12,C,11,C,9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C,19

solasod root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,), x,C,4, [C@@H], 5, ([H]), x, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ring, Ring4, C,15, [C@], 16, ([H]), (,x,O,x, Ring, Ring5,), x, [C@], 17, ([H]), (,x, [C@], 20, (,x, [C@@], 22, Ring, Ring5, (,x,N,x, Ring, Ring6,), x,C,23,C,24, [C@H], 25, (,x,C,26, Ring, Ring6,), x,C,27,), x,C,21,), x, [C@@], 13, Ring, Ring4, (,x,C,18,), x,C,12,C,11,C,9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C,19

furost root steroid

C,3,(,x,C,2,C,1, Ring, Ring1,), x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ring, Ring4, C,15, [C@], 16, ([H]), (,x,O,x, Ring, Ring5,), x, [C@], 17, ([H]), (,x, [C@@], 20, (,x, [C@], 22, Ring, Ring5, C,23,C,24,C,25, (,x,C,26,), x,C,27,), x,C,21,), x, [C@@], 13, Ring, Ring4, (,x,C,18,), x,C,12,C,11,C,9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C,19

chol loveracid steroid

C,1, Ring, Ring1, C,2, [C@H], 3, (O), x,C,4,C,5, Ring, Ring2, C,6, [C@@H], 7, (O), x,C,8, Ring, Ring3, C,14, Ring, Ring4, C,15,C,16, [C@], 17, (,x, [C@@H], 20, (,x,C,22,C,23,C,24,), x,C,21,), x, [C@@], 13, Ring, Ring4, (,x,C,18,), x, [C@@H], 12, (O), x,C,11,C,9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C,19

lithochol loveracid steroid

C,1, Ring, Ring1, C,2, [C@@H], 3, (O), x,C,4,C,5, Ring, Ring2, C,6,C,7,C,8, Ring, Ring3, C,14, Ring, Ring4, C,15,C,16, [C@], 17, (,x, [C@@H], 20, (,x,C,22,C,23,C,24,), x,C,21,), x, [C@@], 13, Ring, Ring4, (,x,C,18,), x,C,12,C,11,C,9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C,19

dehydrochol loveracid steroid

C,1, Ring, Ring1, C, 2, C, 3, (=O), x, C, 4, C, 5, Ring, Ring2, C, 6, C, 7, (=O), x, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, [C@@H], 20, (, x, C, 22, C, 23, C, 24,), x, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, (=O), x, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19

hyodeoxychol loveracid steroid

C,1, Ring, Ring1, C, 2, [C@@H], 3, (O), x, C, 4, C, 5, Ring, Ring2, [C@@H], 6, (O), x, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, [C@@H], 20, (, x, C, 22, C, 23, C, 24,), x, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19

chenodeoxychol loveracid steroid

C,1, Ring, Ring1, C, 2, C, 3, [C@@H], 4, (O), x, C, 5, Ring, Ring2, C, 6, [C@@H], 7, (O), x, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, [C@@H], 20, (, x, C, 22, C, 23, C, 24,), x, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19

ursodeoxychol loveracid steroid

C,1, Ring, Ring1, C, 2, [C@H], 3, (O), x, C, 4, C, 5, Ring, Ring2, C, 6, [C@H], 7, (O), x, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, [C@@H], 20, (, x, C, 22, C, 23, C, 24,), x, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19

tauroursodeoxychol loveracid steroid

S, x, (=O), x, (=O), x, (, x, O, 1@x,), x, C, x, C, x, N, x, Ring, Ring5, ., x, C, 1, Ring, Ring1, C, 2, [C@@H], 3, (O), x, C, 4, C, 5, Ring, Ring2, C, 6, [C@H], 7, (O), x, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, [C@@H], 20, (, x, C, 22, C, 23, C, 24, (=O), x, Ring, Ring5,), x, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, x,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19

taurochol loveracid steroid

S, x, (=O), x, (=O), x, (, x, O, 1@x,), x, C, x, C, x, N, x, Ring, Ring5, ., x, C, 1, Ring, Ring1, C, 2, C, 3, [C@H], 4, (O), x, C, 5, Ring, Ring2, C, 6, [C@@H], 7, (O), x, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, [C@@H], 20, (, x, C, 22, C, 23, C, 24, (=O), x, Ring, Ring5,), x, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, x,), x, [C@@H], 12, (O), x, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19

glycochol loveracid steroid

C,1, Ring, Ring1, C, 2, C, 3, [C@H], 4, (O), x, C, 5, Ring, Ring2, [C@@H], 6, (O), x, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (, x, [C@@H], 20, (, x, C, 22, C, 23, C, 24, (=O)NCC, x,), x, C, 21,), x, [C@@], 13, Ring, Ring4, (, x, C, 18,), x, [C@@H], 12, (O), x, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19

oxymetholone root steroid

C, 3, (=O) (, x, C, 2, (=CO), x, C, 1, Ring, Ring1,), x, C, 4, C, 5, Ring, Ring2, C, 6, C, 7, C, 8, Ring, Ring3, C, 14, Ring, Ring4, C, 15, C, 16, [C@], 17, (O) (C), x, [C@@], 13, Ring, Ring4, (, x, C, x,), x, C, 12, C, 11, C, 9, Ring, Ring3, [C@@], 10, Ring, Ring1, Ring, Ring2, C, 19

homo natderiver nathomo x, x

nor natderiver natnor x, x

seco natderiver natseco x, x

abeo natderiver natabeo x, x

cyclo natderiver cyclo x, x

rightarrow|arrow|fwdarrow|fwdarw unknown natarrow x, x

flophemesyl root root [Si], 4@x, (C) (C) c1c (F) c (F) c (F) c (F) c (F) 1, x

diethylenetriamine root root N, n | 1, C, 2, C, 3, N, n' | 4, C, 5, C, 6, N, n' | 7

triethylenetetramine root root N, n, CC, x, N, n', CC, x, N, n', CC, x, N, n'

tetraethylenepentamine root root

N, n, CC, x, N, n', CC, x, N, n', CC, x, N, n', CC, x, N, n'

pentaethylenhexamine root root

N, n, CC, x, N, n', CC, x, N, n', CC, x, N, n', CC, x, N, n', CC, x, N, n', CC, x, N, n'

cupferron root root O=NN([O-])c1cccc1.[NH4+], x

camphene root root C=C(CC(CC2)C1(C)C)C12C, x

[illegible]

74

Variable	Mean	SD	Min	Max	Median	Q1	Q3	Mode	Skewness	Kurtosis	Shapiro-Wilk	Normality
Age	35.2	12.5	18	65	32	25	40	30	0.15	2.10	0.98	Normal
Gender	1.2	0.4	1	2	1	1	1	1	0.05	0.10	0.95	Normal
Education	12.5	2.1	9	16	12	11	13	12	0.10	1.80	0.99	Normal
Income	4500	1500	2000	8000	4000	3500	5000	4000	0.20	2.50	0.97	Normal
Marital Status	1.5	0.5	1	2	1	1	1	1	0.05	0.10	0.95	Normal
Occupation	2.5	1.2	1	4	2	2	3	2	0.10	1.50	0.98	Normal
Health Status	1.8	0.6	1	2	1	1	1	1	0.05	0.10	0.95	Normal
Stress Level	3.2	1.5	1	5	3	2	4	3	0.15	2.10	0.98	Normal
Life Satisfaction	4.5	1.0	3	6	4	4	5	4	0.10	1.80	0.99	Normal
Work-Life Balance	3.8	1.2	2	5	3	3	4	3	0.15	2.10	0.98	Normal
Family Support	4.2	0.8	3	5	4	4	4	4	0.05	0.10	0.95	Normal
Community Involvement	2.8	1.1	1	4	2	2	3	2	0.10	1.50	0.98	Normal
Personal Growth	3.5	1.3	2	5	3	3	4	3	0.15	2.10	0.98	Normal
Overall Well-being	4.0	0.9	3	5	4	4	4	4	0.05	0.10	0.95	Normal

thioglycol root glycol
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,S,1@x,,x,O,1@x,Ring,Ring1
 dithioglycol root glycol
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,S,1@x,,x,S,1@x,Ring,Ring1
 selenoglycol root glycol
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Se],1@x,,x,O,1@x,Ring,Ring1
 diselenoglycol root glycol
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Se],1@x,,x,[Se],1@x,Ring,Ring1
 telluroglycol root glycol
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Te],1@x,,x,O,1@x,Ring,Ring1
 ditelluroglycol root glycol
 C,1|a|alpha,Ring,Ring1,C,2|b|beta,[Te],1@x,,x,[Te],1@x,Ring,Ring1
 tempo root root
 C,4,Ring,Ring1,C,5,C,6,(C)(C),x,N,1,(x,O,16@x),x,C,2,(C)(C),x,C,3,Ring,Ring1
 proxyl root root
 C,3,Ring,Ring1,C,2,(C)(C),x,N,1,(x,O,16@x),x,C,5,(C)(C),x,C,4,Ring,Ring1
 nitroxide|nitroxyl root root N,n,O,16@x
 nitramine root root N,n,[N+](=O)[O-],x
 nitramino root root N,4@n,[N+](=O)[O-],x
 special-oxine root root
 n,1,Ring,Ring1,c,2|b|beta,c,3,c,4,c,4a,Ring,Ring2,c,5,c,6,c,7,c,8,(O),x,c,8a,Rin
 g,Ring1,Ring,Ring2
 special-azine|ketazine root azine N,8@x,N,8@x
 oxime|oxim|antioxime root oxime N,8@x,O,o
 hydrazone|hydrazon root oxime N,8@x,N,n
 semicarbazone|semicarbazon root oxime N,8@1,N,2,C,3,(=,x,O,x),x,N,4
 azino root bridge N,8@x,N,8@x
 azimino root bridge N,4@x,N,x,=,x,N,4@x
 biimino|biimin root bridge N,4@x,N,4@x
 epidioxy root bridge O,4@x,O,4@x
 epidithio|epidithi root bridge S,4@x,S,4@x
 epimino root bridge N,5@x
 epithio root bridge S,5@x
 episeleno root bridge [Se],5@x
 epitelluro root bridge [Te],5@x
 epithioximino|epithioximin root bridge S,4@x,O,x,N,4@x
 epoxy root bridge O,5@x
 epoxyimino|epoxyimin root bridge O,4@x,N,4@x
 epoxynitrilo root bridge O,4@x,N,8@x
 epoxythio|epoxythi root bridge O,4@x,S,4@x
 epoxythioxy root bridge O,4@x,S,x,O,4@x
 epitritio|epitriti root bridge S,4@x,S,x,S,4@x
 cyanohydrin root oxime O,4@x,,x,C,4@x,#N,x
 fluorohydrin root oxime O,4@x,,x,F,4@x
 chlorohydrin root oxime O,4@x,,x,Cl,4@x
 bromohydrin root oxime O,4@x,,x,Br,4@x
 iodohydrin root oxime O,4@x,,x,I,4@x
 acetal|ketal|semiacetal|demiactal|hemiactal|semiketal|demiketal|hemiketal|glyc
 olacetal|glycolketal root oxime O,4@x,,x,O,4@x
 mercaptal|mercaptole root oxime S,4@x,,x,S,4@x
 ketone|keton root ketone C,x,=,x,O,x
 ketoxime root ketone C,x,=,x,N,x,O,x
 ketoximino root ketone C,x,=,x,N,x,O,4@x
 ketyl root ketone C,4@x,[O-],x
 sulfoxide|sulfoxid root ketone S,x,=,x,O,x
 sulfone|sulfon root ketone S,x,(=,x,O,x),x,=,x,O,x
 sulfimide|sulfimid|sulfilimine|sulfilimin root ketone S,x,=,x,N,x

sulfoximide|sulfoximid|sulfoximine|sulfoximin root ketone
 S,x,(=,x,O,x,),x,=,x,N,x
 selenoxide|selenoxid root ketone [Se],x,=,x,O,x
 selenone|selenon root ketone [Se],x,(=,x,O,x,),x,=,x,O,x
 selenimide|selenimid root ketone [Se],x,=,x,N,x
 selenoximide|selenoximid root ketone [Se],x,(=,x,O,x,),x,=,x,N,x
 telluroxide|telluroxid root ketone [Te],x,=,x,O,x
 tellurone|telluron root ketone [Te],x,(=,x,O,x,),x,=,x,O,x
 tellurimide|tellurimid root ketone [Te],x,=,x,N,x
 telluroximide|telluroximid root ketone [Te],x,(=,x,O,x,),x,=,x,N,x
 peroxide|peroxid root ketone O,x,O,x
 persulfide|persulfid root ketone S,x,S,x
 formal root ketone O,x,Ring,Ring1,.,x,O,x,C,x,Ring,Ring1
 ether root ether O,x
 etherof root ofether O,x
 thioether root ether S,x
 selenoether root ether [Se],x
 telluroether root ether [Te],x
 oin oin unknown C,1@b|beta,(O),x,C,1@a|alpha,=O,x
 ano methanomaker unknown x,x
 quinone|quinon suffix quinone O,8@x
 quinodimethane|quinodimethan suffix quinone C,10@x
 radical radical unknown x,x
 yl suffix yl 1,yl
 ylidene|yliden|ilidene|iliden| suffix yl 2,yl
 ylidyne|ylidyn|ilidyne|ilidyn suffix yl 3,yl
 ane|an suffix ignore x,x
 ine|in suffix ignore x,x
 ene|en suffix bondchange 2,bond
 yne|yn suffix bondchange 3,bond
 thiol|ylthiol suffix suffix S,4@s
 ol suffix olsuffix O,4@x
 olate suffix suffix [O-],4@x
 anethiolate|thiolato suffix suffix [S-],4@x
 one|on suffix reqcarbon O,8@x
 thione suffix reqcarbon S,8@x
 selenone|selone suffix reqcarbon [Se],8@x
 tellurone suffix reqcarbon [Te],8@x
 imine root oxime N,8@n
 imine imine suffix N,8@n
 iminium root oxime [N+],8@x
 iminium imine suffix [N+],8@x
 glycol glycol unknown O,4@o,.,x,O,4@o'
 thioglycol glycol unknown S,4@s,.,x,O,4@o
 dithioglycol glycol unknown S,4@s,.,x,S,4@s'
 selenoglycol glycol unknown [Se],4@x,.,x,O,4@x
 diselenoglycol glycol unknown [Se],4@x,.,x,[Se],4@x
 telluroglycol glycol unknown [Te],4@x,.,x,O,4@x
 ditelluroglycol glycol unknown [Te],4@x,.,x,[Te],4@x
 cyanohydrin glycol unknown C,4@x,#N,x,.,x,O,4@x
 fluorohydrin glycol unknown F,4@x,.,x,O,4@x
 chlorohydrin glycol unknown Cl,4@x,.,x,O,4@x
 bromohydrin glycol unknown Br,4@x,.,x,O,4@x
 iodohydrin glycol unknown I,4@x,.,x,O,4@x
 oxide counterion oxide O,8@x
 sulfide|mercaptide counterion oxide S,8@x
 selenide counterion oxide [Se],8@x

telluride counterion oxide [Te],8@x
 methanoxymethano root methanobridge C,4@x,O,x,C,4@x
 etheno root methanobridge C,4@x,=,x,C,4@x
 metheno root metheno C,5@x
 obenzeno root methanobridge c,4@x,ring,ring1,c,4@x,c,x,c,x,c,x,c,x,ring,ring1
 epoxide|enoxide counterion bridge O,5@x
 episulfide counterion bridge S,5@x
 sultam counterion bridge S,4@x,(=,x,O,x,),x,(=,x,O,x,),x,N,4@x
 sultone|sultone counterion bridge S,4@x,(=,x,O,x,),x,(=,x,O,x,),x,O,4@x
 dicarboximide|dicarboxylicimide|dicarboxylicacidimide counterion bridge
 C,4@x,(=,x,O,x,),x,N,x,C,4@x,=,x,O,x
 dicarboximido counterion bridge
 C,4@x,(=,x,O,x,),x,ring,ring1,.,x,C,4@x,ring,ring2,=,x,O,x,.,x,N,4@x,ring,ring1,
 ring,ring2
 carbolactam counterion bridge C,4@x,(=,x,O,x,),x,O,4@x
 nitride counterion ionable N,12@x
 phosphide counterion ionable P,12@x
 antimonide counterion ionable [Sb],12@x
 arsenide counterion ionable [As],12@x
 hydroxide|hydroxid counterion ionable O,4@x
 deuterioxide|deuteroxid counterion ionable O,4@x,[2H],x
 hydrosulfide|hydrosulfid|sulfhydrate|sulfhydrat counterion ionable S,4@x
 hydroselenide|hydroselenid counterion ionable [Se],4@x
 hydrotelluride|hydrotellurid counterion ionable [Te],4@x
 hydride|hydrid counterion ionable [H],4@1
 deuteride|deuterid counterion ionable [2H],4@1
 fluoride|fluorid counterion ionable F,4@1
 chloride|chlorid|muriate counterion ionable Cl,4@1
 bromide|bromid counterion ionable Br,4@1
 iodide|iodid counterion ionable [I],4@1
 acetylide counterion ionable C,4@x,#[C-],x
 cyanide|cyanid counterion ionable C,4@x,#N,x
 isocyanide|isocyanid|isonitrile counterion ionable [N+],4@x,#[C-],x
 cyanate|cyanat counterion ionable O,4@x,C#N,x
 isocyanate|isocyanat counterion ionable N,4@x,=C=O,x
 fulminate|fulminat counterion ionable O,4@x,[N+]#[C-],x
 thiocyanate|thiocyanat|sulfocyanate|sulfocyanat|sulfocyanide|sulfocyanid|rhodani
 de|rhodanid counterion ionable S,4@x,C#N,x
 isothiocyanate|isothiocyanat|isorhodanide|isorhodanid counterion ionable
 N,4@x,=C=S,x
 selenocyanate|selenocyanat counterion ionable [Se],4@x,C#N,x
 isoselenocyanate|isoselenocyanat counterion ionable N,4@x,=C=[Se],x
 tellurocyanate|tellurocyanat counterion ionable [Te],4@x,C#N,x
 isotellurocyanate|isotellurocyanat counterion ionable N,4@x,=C=[Te],x
 azide|azid counterion ionable N,4@x,=[N+]=[N-],x
 sulfenamide|sulfenamid counterion counterion S,4@x,N,n
 sulfonazide counterion counterion S,4@x,(=O)(=O)N[N+][N-],x
 alcohol|icalcohol counterion counterion O,4@x
 deuterol counterion counterion O,4@x,[2H],x
 selenol counterion counterion [Se],4@s
 tellurol counterion counterion [Te],4@s
 nitrile|nitril counterion counterion N,12@x
 carbonitrile|carbonitril counterion counterion C#N,4@x
 diazonium counterion counterion [N+],4@x,#N,x
 mercaptan|thioalcohol counterion counterion S,4@x
 hydroperoxide|hydroperoxid counterion ionable O,4@x,O,x

[illegible]

hexali|hexalia prefix chainable 6000,mult
 heptali|heptalia prefix chainable 7000,mult
 octali|octalia prefix chainable 8000,mult
 nonali|nonalia prefix chainable 9000,mult
 cyclo cyclo cyclo 1,cyclo
 spiro spiro unknown 1,spiro

onia chargegiver replacement 1,charge
 onium chargegiver root 1,charge
 onio chargegiver infix 1,charge
 ium|iumion|iumcation chargegiver trivial 1,charge
 ide|ideion|ideanion chargegiver trivial -1,charge
 cation|ylium|ylcation suffix namedcharge 1,charge
 anion|ylide|ylanion suffix namedcharge -1,charge
 ion suffix namedcharge 0,charge

oxammonium root root 0,x,[N+],x
 ammonium|aminium root root [N+],n|omega
 ammonio infix infix [N+],4@n
 phosphonium root root [P+],x|omega
 phosphonio infix infix [P+],4@x
 arsonium root root [As+],x|omega
 arsonio infix infix [As+],4@x
 stibonium root root [Sb+],x|omega
 stibonio infix infix [Sb+],4@x
 bismuthonium root root [Bi+],x|omega
 bismuthonio infix infix [Bi+],4@x
 sulfonium root root [S+],s|omega
 selenonium root root [Se+],s|omega
 telluronium root root [Te+],s|omega
 sulfoxonium root root [S+],s,=O,x
 sulfonio infix infix [S+],4@s
 chloronium root root [Cl+],x|omega
 chloronio infix infix [Cl+],4@x
 bromonium root root [Br+],x|omega
 bromonio infix infix [Br+],4@x
 iodonium root root [I+],x|omega
 iodonio infix infix [I+],4@x

actina replacement replacement [Ac],x
 alumina|alumin replacement replacement [Al],x
 argenta|argent replacement replacement [Ag],x
 arsa|ars|arsen replacement replacement [As],x
 arsora|arsor replacement replacement [AsH5],x
 astata|astat replacement replacement [At],x
 aura replacement replacement [Au],x
 aza|az replacement replacement N,n
 bara replacement replacement [Ba],x
 berkela|berkel replacement replacement [Bk],x
 berylla|beryll replacement replacement [Be],x
 bisma|bism replacement replacement [Bi],x
 bora|bor replacement replacement [B],x
 broma replacement replacement [Br],x
 cadma|cadm replacement replacement [Cd],x
 calca|calc replacement replacement [Ca],x
 californa|californ replacement replacement [Cf],x
 carba|carb replacement replacement [C],x

Gene	Accession	Length (bp)	GC (%)	GC (3rd pos) (%)	GC (4th pos) (%)	GC (5th pos) (%)	GC (6th pos) (%)	GC (7th pos) (%)	GC (8th pos) (%)	GC (9th pos) (%)	GC (10th pos) (%)	GC (11th pos) (%)	GC (12th pos) (%)	GC (13th pos) (%)	GC (14th pos) (%)	GC (15th pos) (%)	GC (16th pos) (%)	GC (17th pos) (%)	GC (18th pos) (%)	GC (19th pos) (%)	GC (20th pos) (%)	GC (21st pos) (%)	GC (22nd pos) (%)	GC (23rd pos) (%)	GC (24th pos) (%)	GC (25th pos) (%)	GC (26th pos) (%)	GC (27th pos) (%)	GC (28th pos) (%)	GC (29th pos) (%)	GC (30th pos) (%)	GC (31st pos) (%)	GC (32nd pos) (%)	GC (33rd pos) (%)	GC (34th pos) (%)	GC (35th pos) (%)	GC (36th pos) (%)	GC (37th pos) (%)	GC (38th pos) (%)	GC (39th pos) (%)	GC (40th pos) (%)	GC (41st pos) (%)	GC (42nd pos) (%)	GC (43rd pos) (%)	GC (44th pos) (%)	GC (45th pos) (%)	GC (46th pos) (%)	GC (47th pos) (%)	GC (48th pos) (%)	GC (49th pos) (%)	GC (50th pos) (%)	GC (51st pos) (%)	GC (52nd pos) (%)	GC (53rd pos) (%)	GC (54th pos) (%)	GC (55th pos) (%)	GC (56th pos) (%)	GC (57th pos) (%)	GC (58th pos) (%)	GC (59th pos) (%)	GC (60th pos) (%)	GC (61st pos) (%)	GC (62nd pos) (%)	GC (63rd pos) (%)	GC (64th pos) (%)	GC (65th pos) (%)	GC (66th pos) (%)	GC (67th pos) (%)	GC (68th pos) (%)	GC (69th pos) (%)	GC (70th pos) (%)	GC (71st pos) (%)	GC (72nd pos) (%)	GC (73rd pos) (%)	GC (74th pos) (%)	GC (75th pos) (%)	GC (76th pos) (%)	GC (77th pos) (%)	GC (78th pos) (%)	GC (79th pos) (%)	GC (80th pos) (%)	GC (81st pos) (%)	GC (82nd pos) (%)	GC (83rd pos) (%)	GC (84th pos) (%)	GC (85th pos) (%)	GC (86th pos) (%)	GC (87th pos) (%)	GC (88th pos) (%)	GC (89th pos) (%)	GC (90th pos) (%)	GC (91st pos) (%)	GC (92nd pos) (%)	GC (93rd pos) (%)	GC (94th pos) (%)	GC (95th pos) (%)	GC (96th pos) (%)	GC (97th pos) (%)	GC (98th pos) (%)	GC (99th pos) (%)	GC (100th pos) (%)
Gene 1	Accession 1	Length 1	GC 1	GC 3rd pos 1	GC 4th pos 1	GC 5th pos 1	GC 6th pos 1	GC 7th pos 1	GC 8th pos 1	GC 9th pos 1	GC 10th pos 1	GC 11th pos 1	GC 12th pos 1	GC 13th pos 1	GC 14th pos 1	GC 15th pos 1	GC 16th pos 1	GC 17th pos 1	GC 18th pos 1	GC 19th pos 1	GC 20th pos 1	GC 21st pos 1	GC 22nd pos 1	GC 23rd pos 1	GC 24th pos 1	GC 25th pos 1	GC 26th pos 1	GC 27th pos 1	GC 28th pos 1	GC 29th pos 1	GC 30th pos 1	GC 31st pos 1	GC 32nd pos 1	GC 33rd pos 1	GC 34th pos 1	GC 35th pos 1	GC 36th pos 1	GC 37th pos 1	GC 38th pos 1	GC 39th pos 1	GC 40th pos 1	GC 41st pos 1	GC 42nd pos 1	GC 43rd pos 1	GC 44th pos 1	GC 45th pos 1	GC 46th pos 1	GC 47th pos 1	GC 48th pos 1	GC 49th pos 1	GC 50th pos 1	GC 51st pos 1	GC 52nd pos 1	GC 53rd pos 1	GC 54th pos 1	GC 55th pos 1	GC 56th pos 1	GC 57th pos 1	GC 58th pos 1	GC 59th pos 1	GC 60th pos 1	GC 61st pos 1	GC 62nd pos 1	GC 63rd pos 1	GC 64th pos 1	GC 65th pos 1	GC 66th pos 1	GC 67th pos 1	GC 68th pos 1	GC 69th pos 1	GC 70th pos 1	GC 71st pos 1	GC 72nd pos 1	GC 73rd pos 1	GC 74th pos 1	GC 75th pos 1	GC 76th pos 1	GC 77th pos 1	GC 78th pos 1	GC 79th pos 1	GC 80th pos 1	GC 81st pos 1	GC 82nd pos 1	GC 83rd pos 1	GC 84th pos 1	GC 85th pos 1	GC 86th pos 1	GC 87th pos 1	GC 88th pos 1	GC 89th pos 1	GC 90th pos 1	GC 91st pos 1	GC 92nd pos 1	GC 93rd pos 1	GC 94th pos 1	GC 95th pos 1	GC 96th pos 1	GC 97th pos 1	GC 98th pos 1	GC 99th pos 1	GC 100th pos 1

83

thiolacton|thiolactone part2acid lactone S,5@x
selenolacton|selenolactone part2acid lactone [Se],5@x
tellurolacton|tellurolactone part2acid lactone [Te],5@x
lacton|lactone|olacton|olactone|iclacton|iclactone|olide|olid acid lactone
O,8@x,,x,O,5@x
lactam part2acid lactone N,5@x
lactam|olactam|iclactam acid lactone O,8@x,,x,N,5@x
lactim part2acid lactone N,9@x
lactim|olactim|iclactim acid lactone O,4@x,,x,N,9@x
sulfimide part2acid lactone N,4@x,S,1@x,(=O)(=O),x
anilide|analide acid acid
O,8@x,,x,N,4@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1),
x
anilide|analide part2acid amide
N,4@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1),x
anilido|analido acid infix
O,8@x,,x,N,5@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1),
x
anilido|analido part2acid infix
N,5@n,(,x,c,1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1),x
4nitroanilide|pnitroanilide acid acid
O,8@x,,x,N,4@n,(,x,c,1',Ring,Ring1,c,2',c,3',c,4',([N+](=O)[O-
]),x,c,5',c,6',Ring,Ring1),x
4nitroanilide|pnitroanilide part2acid acid
N,4@n,(,x,c,1',Ring,Ring1,c,2',c,3',c,4',([N+](=O)[O-
]),x,c,5',c,6',Ring,Ring1),x
morpholide acid acid O,8@x,,x,N,4@x,Ring,Ring1,C,x,C,x,O,x,C,x,C,x,Ring,Ring1
morpholide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,O,x,C,x,C,x,Ring,Ring1
ophenone acid acid
O,8@x,,x,c,4@1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1
ophenone part2acid acid
c,4@1',Ring,Ring1,c,2'|o,c,3'|m,c,4'|p,c,5',c,6',Ring,Ring1
onaphthone acid acid
O,8@x,,x,c,4@1',Ring,Ring1,c,2',c,3',c,4',c,4a',Ring,Ring2,c,5',c,6',c,7',c,8',
c,8a',Ring,Ring1,Ring,Ring2
onaphthone part2acid acid
c,4@1',Ring,Ring1,c,2',c,3',c,4',c,4a',Ring,Ring2,c,5',c,6',c,7',c,8',c,8a',Ring
,Ring1,Ring,Ring2
ureide acid acid O,8@x,,x,N,4@n,C(=O),x,N,n'
ureide part2acid amide N,4@n,C(=O),x,N,n'
piperazide acid acid O,8@x,,x,N,4@x,Ring,Ring1,C,x,C,x,N,x,C,x,C,x,Ring,Ring1
piperazide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,N,x,C,x,C,x,Ring,Ring1
piperidide acid acid O,8@x,,x,N,4@x,Ring,Ring1,C,x,C,x,C,x,C,x,C,x,Ring,Ring1
piperidide part2acid acid N,4@x,Ring,Ring1,C,x,C,x,C,x,C,x,C,x,Ring,Ring1
anhydride|cyclicanhydride part2acid anhydride O,5@x
thioanhydride part2acid anhydride S,5@x
selenoanhydride part2acid anhydride [Se],5@x
telluroanhydride part2acid anhydride [Te],5@x
imid|imide part2acid anhydride N,5@x
cyclam root root S,x,(=O)(=O),x,(NC1CCCC1),x,O,1@x
atrop loveracid root
C,x,C,x,(,x,=,x,C,x),x,c,1,Ring,Ring1,c,2|o|ortho,c,3|m|meta,c,4|p|para,c,5,c,6
,Ring,Ring1
pinon loveracid root CCC1CC(C(C)(C)1)C(=O)C,x
benzil loveracid root
C,x,C,a|alpha,(,x,O,x),x,(,x,c,1,Ring,Ring1,=,x,c,2,c,3,c,4,c,5,c,6,Ring,Ring1,
),x,c,1',Ring,Ring2,c,2',c,3',c,4',c,5',c,6',Ring,Ring2

glycoll|glycol loveracid alkane C,x,C,2|w|omega,0,x
thioglycoll|thioglycol loveracid root C,x,C,2,S,w|omega
selenoglycoll|selenoglycol loveracid root C,x,C,2,[Se],w|omega
telluroglycoll|telluroglycol loveracid root C,x,C,2,[Te],w|omega
boro|bor|orthobor loveracid root [B],x,(,x,O,1@o'',),x,(,x,O,1@o',),x,O,1@o
metabor loveracid root [B],x,(,x,=,x,O,o',),x,O,1@o
perbor loveracid root [B],x,(,x,=,x,O,x),(,x,=,x,O,x),x,O,1@o
borin loveracid root [B],x,O,1@o
borono|boron loveracid counterion [B],4@x,(,x,O,1@o',),x,O,1@o
diphosphor|pyrophosphor|pyrophosph loveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o'',),(,x,O,1@o'|p1,),x,O,x,P,b|beta,(=,x,O,x),(,x,O,1@o''''|p2,),x,O,1@o''''
dithiodiphosphor|dithiopyrophosphor|dithiopyrophosph loveracid root
P,a|alpha,(=,x,S,x),(,x,O,1@o'',),(,x,O,1@o'|p1,),x,O,x,P,b|beta,(=,x,S,x),(,x,O,1@o''''|p2,),x,O,1@o''''
phosphosulf loveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o'',),(,x,O,1@o',),x,O,x,S,b|beta,(=,x,O,x),(=,x,O,x),x,O,1@o''''
glycerophosph|alphaglycerophosph|lalphaglycerophosph|dalphaglycerophosph|dlalpha
glycerophosph loveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o'',),(,x,O,1@o',),x,OCC(O)CO,x
glycerophospho|alphaglycerophospho|lalphaglycerophospho|dalphaglycerophospho|dla
lphaglycerophospho loveracid root
P,4@a|alpha,(=,x,O,x),(,x,O,1@o',),x,OCC(O)CO,x
triphosphor loveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o'',),(,x,O,1@o'|p1,),x,O,x,P,b|beta,(=,x,O,x),(,x,O,1@o''''|p2,),x,O,x,P,g|gamma,(=,x,O,x),(,x,O,1@o''''',),x,O,1@o''''''|p3
2thiodiphosphor loveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o'',),(,x,O,1@o'|p1,),x,O,x,P,b|beta,(=,x,S,x),(,x,O,1@o''''|p2,),x,O,1@o''''
3thiotriphosphor loveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o'',),(,x,O,1@o'|p1,),x,O,x,P,b|beta,(=,x,O,x),(,x,O,1@o''''|p2,),x,O,x,P,g|gamma,(=,x,S,x),(,x,O,1@o''''',),x,O,1@o''''''|p3
tetraphosphor loveracid root
P,a|alpha,(=,x,O,x),(,x,O,1@o'',),(,x,O,1@o'|p1,),x,O,x,P,b|beta,(=,x,O,x),(,x,O,1@o''''|p2,),x,O,x,P,g|gamma,(=,x,O,x),(,x,O,1@o''''',),x,O,o''''''|p3,P,d|delta,(=,x,O,x),(,x,O,1@o''''''',),x,O,1@o''''''''|p4
phosphoro|phosphor|phosph|orthophosph|orthophosphor loveracid root
P,x,(=,x,O,x),(,x,O,1@o'',),(,x,O,1@o',),x,O,1@o
phosphono|phosphon loveracid counterion P,4@x,(=,x,O,x),(,x,O,1@o',),x,O,1@o
phospheno|phosphen loveracid root P,x,(=,x,O,x),(=,x,O,x),x,O,1@o
hypophosph loveracid root [PH0],x,(=,x,O,x),(=,x,O,x),x,O,1@o
phosphino|phosphin loveracid root [PH2],x,(=,x,O,x),x,O,1@o
phosphoenolpyruv loveracid root
P,x,(=,x,O,x),(,x,O,1@o',),(,x,O,1@o,),x,O,x,C,x,(=C),x,C,x,(=O),x,O,1@x
phyt loveracid root
O=P(,x,O,1@x),(,x,O,1@x),O[C@H]1[C@@H](OP(,x,O,1@x),(,x,O,1@x,)=O)[C@@H](OP(,x,O,1@x),(,x,O,1@x,)=O)[C@H](OP(,x,O,1@x),(,x,O,1@x,)=O)[C@@H](OP(,x,O,1@x),(,x,O,1@x,)=O)[C@@H]1OP(,x,O,1@x),(,x,O,1@x,)=O,x
orthoarsen|arseno|arsen loveracid root
[As],x,(=,x,O,x),(,x,O,1@o'',),(,x,O,1@o',),x,O,1@o
arsenicacid root root [As],x,(=,x,O,x),(,x,O,1@o'',),(,x,O,1@o',),x,O,1@o
arsono|arson loveracid counterion [As],4@x,(=,x,O,x),(,x,O,1@o',),x,O,1@o
arsino|arsin loveracid root [AsH2],x,(=,x,O,x),x,O,1@o
stibeno|stiben|antimon loveracid root
[Sb],x,(=,x,O,x),(,x,O,1@o'',),(,x,O,1@o',),x,O,1@o
stibono|stibon loveracid counterion [Sb],4@x,(=,x,O,x),(,x,O,1@o',),x,O,1@o

Variable	1990		1995		2000		2005		2010		2015		2020		2025		2030		2035		2040		2045		2050																																																																																																																																																																																																																																																																																																																																																							
	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD	Mean	SD																																																																																																																																																																																																																																																																																																																																																						
Age	25.5	1.2	26.5	1.3	27.5	1.4	28.5	1.5	29.5	1.6	30.5	1.7	31.5	1.8	32.5	1.9	33.5	2.0	34.5	2.1	35.5	2.2	36.5	2.3	37.5	2.4	38.5	2.5	39.5	2.6	40.5	2.7	41.5	2.8	42.5	2.9	43.5	3.0	44.5	3.1	45.5	3.2	46.5	3.3	47.5	3.4	48.5	3.5	49.5	3.6	50.5	3.7	51.5	3.8	52.5	3.9	53.5	4.0	54.5	4.1	55.5	4.2	56.5	4.3	57.5	4.4	58.5	4.5	59.5	4.6	60.5	4.7	61.5	4.8	62.5	4.9	63.5	5.0	64.5	5.1	65.5	5.2	66.5	5.3	67.5	5.4	68.5	5.5	69.5	5.6	70.5	5.7	71.5	5.8	72.5	5.9	73.5	6.0	74.5	6.1	75.5	6.2	76.5	6.3	77.5	6.4	78.5	6.5	79.5	6.6	80.5	6.7	81.5	6.8	82.5	6.9	83.5	7.0	84.5	7.1	85.5	7.2	86.5	7.3	87.5	7.4	88.5	7.5	89.5	7.6	90.5	7.7	91.5	7.8	92.5	7.9	93.5	8.0	94.5	8.1	95.5	8.2	96.5	8.3	97.5	8.4	98.5	8.5	99.5	8.6	100.5	8.7	101.5	8.8	102.5	8.9	103.5	9.0	104.5	9.1	105.5	9.2	106.5	9.3	107.5	9.4	108.5	9.5	109.5	9.6	110.5	9.7	111.5	9.8	112.5	9.9	113.5	10.0	114.5	10.1	115.5	10.2	116.5	10.3	117.5	10.4	118.5	10.5	119.5	10.6	120.5	10.7	121.5	10.8	122.5	10.9	123.5	11.0	124.5	11.1	125.5	11.2	126.5	11.3	127.5	11.4	128.5	11.5	129.5	11.6	130.5	11.7	131.5	11.8	132.5	11.9	133.5	12.0	134.5	12.1	135.5	12.2	136.5	12.3	137.5	12.4	138.5	12.5	139.5	12.6	140.5	12.7	141.5	12.8	142.5	12.9	143.5	13.0	144.5	13.1	145.5	13.2	146.5	13.3	147.5	13.4	148.5	13.5	149.5	13.6	150.5	13.7	151.5	13.8	152.5	13.9	153.5	14.0	154.5	14.1	155.5	14.2	156.5	14.3	157.5	14.4	158.5	14.5	159.5	14.6	160.5	14.7	161.5	14.8	162.5	14.9	163.5	15.0	164.5	15.1	165.5	15.2	166.5	15.3	167.5	15.4	168.5	15.5	169.5	15.6	170.5	15.7	171.5	15.8	172.5	15.9	173.5	16.0	174.5	16.1	175.5	16.2	176.5	16.3	177.5	16.4	178.5	16.5	179.5	16.6	180.5	16.7	181.5	16.8	182.5	16.9	183.5	17.0	184.5	17.1	185.5	17.2	186.5	17.3	187.5	17.4	188.5	17.5	189.5	17.6	190.5	17.7	191.5	17.8	192.5	17.9	193.5	18.0	194.5	18.1	195.5	18.2	196.5	18.3	197.5	18.4	198.5	18.5	199.5	18.6	200.5	18.7	201.5	18.8	202.5	18.9	203.5	19.0	204.5	19.1	205.5	19.2	206.5	19.3	207.5	19.4	208.5	19


```
benzin nothandled nothandled x,x
dodecin nothandled nothandled x,x
methin nothandled nothandled x,x
- nothandled nothandled x,x
tolane nothandled nothandled x,x
monocrotaline nothandled nothandled x,x
adiphenine nothandled nothandled x,x
anhydridewith nothandled nothandled x,x
terpin nothandled nothandled x,x
thiuram nothandled nothandled x,x
acaprazine nothandled unknown x,x
acaralate nothandled unknown x,x
acetazide nothandled unknown x,x
acetazolamide root root CC(NC1=NN=C(S(N)(=O)=O)S1)=O,x
acetene nothandled unknown x,x
acetoexamide nothandled unknown x,x
acetonyl nothandled unknown x,x
aconitine nothandled unknown x,x
alipamide nothandled unknown x,x
ambrosin nothandled unknown x,x
amygdalin nothandled unknown x,x
anisene nothandled unknown x,x
anisindione nothandled unknown x,x
antichlor nothandled unknown x,x
antiethanol nothandled unknown x,x
antiformin nothandled unknown x,x
antiphen nothandled unknown x,x
arsamin nothandled unknown x,x
arsenal nothandled unknown x,x
arsenolite nothandled unknown x,x
atolide nothandled unknown x,x
azamethone nothandled unknown x,x
azinthiamide nothandled unknown x,x
azobutyl nothandled unknown x,x
azolimine nothandled unknown x,x
azopyrin nothandled unknown x,x
benzilan nothandled unknown x,x
benzilen nothandled unknown x,x
benzylene nothandled unknown x,x
benzolin nothandled unknown x,x
benzone nothandled unknown x,x
benzoxonium nothandled unknown x,x
benztropine|benzotropine root root CN3C4CC(CC3CC4)OC(C2=CC=CC=C2)C1=CC=CC=C1,x
biamine nothandled unknown x,x
bichlorendo nothandled unknown x,x
biclofibrate nothandled unknown x,x
biformylchlorazin nothandled unknown x,x
biphenate nothandled unknown x,x
bisoxypyphen nothandled unknown x,x
blauramine nothandled unknown x,x
borolin nothandled unknown x,x
boroxine nothandled unknown x,x
bromacrylide nothandled unknown x,x
bromamide nothandled unknown x,x
bromethalin nothandled unknown x,x
bromhexine root root CN(C2CCCCC2)CC1=C(N)C(Br)=CC(Br)=C1,x
brominal nothandled unknown x,x
```

[illegible]

[illegible]

Gene	Accession	Length (bp)	GC (%)	GC (3rd pos) (%)	GC (4th pos) (%)	GC (5th pos) (%)	GC (6th pos) (%)	GC (7th pos) (%)	GC (8th pos) (%)	GC (9th pos) (%)	GC (10th pos) (%)	GC (11th pos) (%)	GC (12th pos) (%)	GC (13th pos) (%)	GC (14th pos) (%)	GC (15th pos) (%)	GC (16th pos) (%)	GC (17th pos) (%)	GC (18th pos) (%)	GC (19th pos) (%)	GC (20th pos) (%)	GC (21st pos) (%)	GC (22nd pos) (%)	GC (23rd pos) (%)	GC (24th pos) (%)	GC (25th pos) (%)	GC (26th pos) (%)	GC (27th pos) (%)	GC (28th pos) (%)	GC (29th pos) (%)	GC (30th pos) (%)	GC (31st pos) (%)	GC (32nd pos) (%)	GC (33rd pos) (%)	GC (34th pos) (%)	GC (35th pos) (%)	GC (36th pos) (%)	GC (37th pos) (%)	GC (38th pos) (%)	GC (39th pos) (%)	GC (40th pos) (%)	GC (41st pos) (%)	GC (42nd pos) (%)	GC (43rd pos) (%)	GC (44th pos) (%)	GC (45th pos) (%)	GC (46th pos) (%)	GC (47th pos) (%)	GC (48th pos) (%)	GC (49th pos) (%)	GC (50th pos) (%)
Gene 1	Accession 1	Length 1	GC 1	GC 3rd pos 1	GC 4th pos 1	GC 5th pos 1	GC 6th pos 1	GC 7th pos 1	GC 8th pos 1	GC 9th pos 1	GC 10th pos 1	GC 11th pos 1	GC 12th pos 1	GC 13th pos 1	GC 14th pos 1	GC 15th pos 1	GC 16th pos 1	GC 17th pos 1	GC 18th pos 1	GC 19th pos 1	GC 20th pos 1	GC 21st pos 1	GC 22nd pos 1	GC 23rd pos 1	GC 24th pos 1	GC 25th pos 1	GC 26th pos 1	GC 27th pos 1	GC 28th pos 1	GC 29th pos 1	GC 30th pos 1	GC 31st pos 1	GC 32nd pos 1	GC 33rd pos 1	GC 34th pos 1	GC 35th pos 1	GC 36th pos 1	GC 37th pos 1	GC 38th pos 1	GC 39th pos 1	GC 40th pos 1	GC 41st pos 1	GC 42nd pos 1	GC 43rd pos 1	GC 44th pos 1	GC 45th pos 1	GC 46th pos 1	GC 47th pos 1	GC 48th pos 1	GC 49th pos 1	GC 50th pos 1
Gene 2	Accession 2	Length 2	GC 2	GC 3rd pos 2	GC 4th pos 2	GC 5th pos 2	GC 6th pos 2	GC 7th pos 2	GC 8th pos 2	GC 9th pos 2	GC 10th pos 2	GC 11th pos 2	GC 12th pos 2	GC 13th pos 2	GC 14th pos 2	GC 15th pos 2	GC 16th pos 2	GC 17th pos 2	GC 18th pos 2	GC 19th pos 2	GC 20th pos 2	GC 21st pos 2	GC 22nd pos 2	GC 23rd pos 2	GC 24th pos 2	GC 25th pos 2	GC 26th pos 2	GC 27th pos 2	GC 28th pos 2	GC 29th pos 2	GC 30th pos 2	GC 31st pos 2	GC 32nd pos 2	GC 33rd pos 2	GC 34th pos 2	GC 35th pos 2	GC 36th pos 2	GC 37th pos 2	GC 38th pos 2	GC 39th pos 2	GC 40th pos 2	GC 41st pos 2	GC 42nd pos 2	GC 43rd pos 2	GC 44th pos 2	GC 45th pos 2	GC 46th pos 2	GC 47th pos 2	GC 48th pos 2	GC 49th pos 2	GC 50th pos 2

morinamide nothandled unknown x,x
 naphthonone nothandled unknown x,x
 neonal nothandled unknown x,x
 neophan nothandled unknown x,x
 neraminol nothandled unknown x,x
 nicetal nothandled unknown x,x
 nicetamide nothandled unknown x,x
 nitralin nothandled unknown x,x
 nitrochlor nothandled unknown x,x
 nitroglycerin nothandled unknown x,x
 nitroglycerol nothandled unknown x,x
 octatropine nothandled unknown x,x
 ophthalmamin nothandled unknown x,x
 oxaine nothandled unknown x,x
 oxamyl nothandled unknown x,x
 oxanamide nothandled unknown x,x
 oxanilide nothandled unknown x,x
 oxanthrene nothandled unknown x,x
 oxolamine root root CCN(CCC1=NC(C2=CC=CC=C2)=NO1)CC,x
 oxophenarsine nothandled unknown x,x
 oxoprostol nothandled unknown x,x
 oxybutynin root root CCN(CC#CCOC(C(C1CCCCC1)(c2ccccc2)O)=O)CC,x
 oxydiazol nothandled unknown x,x
 oxyfume nothandled unknown x,x
 oxylan nothandled unknown x,x
 oxylite nothandled unknown x,x
 pentalenene nothandled unknown x,x
 pentalenolactone nothandled unknown x,x
 pentanochlor nothandled unknown x,x
 pernitr nothandled unknown x,x
 persilic nothandled unknown x,x
 phenactropinium nothandled unknown x,x
 phenatine nothandled unknown x,x
 phenatoine nothandled unknown x,x
 phenazon nothandled unknown x,x
 phenformin root root N=C(NC(N)=N)NCCCC1=CC=CC=C1,x
 phenonyl nothandled unknown x,x
 phenoxethol nothandled unknown x,x
 phenoxybenzamine nothandled unknown x,x
 phenoxytol nothandled unknown x,x
 phenvalerate nothandled unknown x,x
 phloretin root root O=C(CCC2=CC=C(O)C=C2)C1=C(O)C=C(O)C=C1O,x
 phosphaniline nothandled unknown x,x
 phosphestrol nothandled unknown x,x
 phosphotrienin nothandled unknown x,x
 phthalazinol nothandled unknown x,x
 phytin nothandled unknown x,x
 pinacolin nothandled unknown x,x
 piperazate nothandled unknown x,x
 piperidolate root root O=C(OC2CN(CC)CCC2)C(C3=CC=CC=C3)C1=CC=CC=C1,x
 pivalone nothandled unknown x,x
 pivalyn nothandled unknown x,x
 propal nothandled unknown x,x
 propamide nothandled unknown x,x
 propargite nothandled unknown x,x
 propazolamide nothandled unknown x,x
 propiodal nothandled unknown x,x

[illegible]

each|electrolytic|electronic|electrophoresis|environmental|esterification|extrac
 tion|extrapure stopword toend x,x
 fcc|filings|fine|finest|flake|flakes|fluorescent|fluorimetric|foil|for|freeradic
 al|from|fume stopword toend x,x
 gas|gauze|gcstandard|glacial|granular|granulate|granule|granules stopword toend
 x,x
 heavy|hplc|hydrophobic stopword toend x,x
 indicator|ingot|ingots|iupac stopword toend x,x
 light|liquid|loose|low|lump|lumps stopword toend x,x
 mainly|maycontain|metal|metals|minimum|moist|mossy stopword toend x,x
 native|natural|needle|needles|notstabilized stopword toend x,x
 on|onactivatedcarbon|optical|organic stopword toend x,x
 particle|pearl|pearls|pellet|pellets|photopolymerization|piece|pieces|plasticize
 r stopword toend x,x
 plate|plates|porous|powder|pract|practical|predominantly|predominatly|primarysta
 ndard|puratronic|pure|purum stopword toend x,x
 reagent|reagentfor|reagentacs|redox|reference|remainder|research|ribbon|ribbons|
 rod|rods stopword toend x,x
 scale|scales|scoop|secondarystandard|selective|sensitive|shaving|shavings|shot
 stopword toend x,x
 simultaneous|singlecrystal|slug|slugs|soft|solid|solution|soot|spectrographic|sp
 ectrophotometric stopword toend x,x
 sphere|spheres|spin|sponge|spray|stab|stabilized|stable|standard|stick|sticks|su
 spension|synthetic|syrup|syrupy stopword toend x,x
 tablet|tablets|tech|technical|thinfoil|titrant|topical|turnings|typically
 stopword toend x,x
 ultra|ultrapure|unstabilized|ultrathinfoil|usp|uvgrade stopword toend x,x
 vial|volumetricstandard stopword toend x,x
 wet|wire|wires|wool stopword toend x,x
 zonerefined stopword toend x,x
 24d|245t|24dnp buildable unknown x,x
 thinfoil|ultrathinfoil|singlecrystal buildable unknown x,x
 antibovine|anticat|antichicken|antidog|antigoat|antiguineapig|antihorse|antihuma
 n|antimonkey|antirabbit|antirat|antisheep notthisversion macromolecule x,x
 tetrahydroprogesterone|tetrahydroprogesteron buildable unknown x,x
 hydrofluoride|hydrochloride|methochloride|methobromide|hydrobromide|hydroiodide|
 hydriodide|methiodide|methiodide|ethiodide|ethiodide buildable unknown x,x
 cyclopentadefphenanthren|cyclopentadefphenanthrene buildable unknown x,x
 1011dihydrocinchon|1011dihydrocinchonine|1011dihydrocinchonin|1011dihydroquinidi
 ne|1011dihydrocinchonidine|1011dihydrocinchonidin buildable unknown x,x
 1011dihydroquinine|1011dihydroquinin|dihydroquinine|dihydroquinin|hydroquinine|h
 ydroquinin buildable unknown x,x
 alphaergocryptine|alphaergocryptin|alphaergocriptine|alphaergocriptin buildable
 unknown x,x
 betaergocryptine|betaergocryptin|betaergocriptine|betaergocriptin|bergocryptine|
 bergocryptin|bergocriptine|bergocriptin buildable unknown x,x
 alphaergocryptinine|alphaergocryptinin|alphaergocriptinine|alphaergocriptinin
 buildable unknown x,x
 betaergocryptinine|betaergocryptinin|betaergocriptinine|betaergocriptinin|bergoc
 riptinine|bergocryptinin|bergocriptinine|bergocriptinin buildable unknown x,x
 1alphah5alphahtropan buildable unknown x,x
 ethylvanillin|ethylcitral buildable unknown x,x
 orthocatechol buildable unknown x,x
 isatoicanhydride buildable unknown x,x
 cresylicacid buildable unknown x,x
 chlorosulfamicacid buildable unknown x,x

hexafluorophosphoricacid|hexafluorosilicicacid|hexafluorozirconicacid|tetraflu
 oroboricacid buildable unknown x,x
 ylcation|ylanion buildable unknown x,x
 betaalan buildable unknown x,x
 crotonylalcohol buildable unknown x,x
 betainealdehyde|betainaldehyd buildable unknown x,x
 biotinamide|biotinamid buildable unknown x,x
 angeldust buildable unknown x,x
 catecholborane buildable unknown x,x
 vitaminb1nitrate|thiaminenitrate|thiaminnitrate|thiaminechloride|thiaminchlorid
 buildable unknown x,x
 44'carbocyanine|22'carbocyanine buildable unknown x,x
 ylthiol buildable unknown x,x
 benzeneoxid|benzeneoxide buildable unknown x,x
 card|2022cardenolide|card2022enolide buildable unknown x,x
 25norbornadien|25norbornadiene|2norbornene|2norbornen|5norbornene|5norbornen
 buildable unknown x,x
 icalcohol buildable unknown x,x
 orthophthal buildable unknown x,x
 neopentylglycol buildable unknown x,x
 nitrogendioxide|nitricoxide|nitrousoxide buildable unknown x,x
 hydrogenphosphato|dihydrogenphosphato buildable unknown x,x
 chloralhydrate|bromalhydrate buildable unknown x,x
 vinylsulfurol buildable unknown x,x
 arsenicacid buildable unknown x,x
 methacr buildable unknown x,x
 formamidinedisulfide buildable unknown x,x
 isonitroso|isonitros|isonipecot|isobenzofuran|isocrotono|isocroton|isocrot|isoqu
 inol|isochinol|glutathionerduced buildable unknown x,x
 3thiotriphosphor|2thiodiphosphor buildable unknown x,x
 alphalinolen|gammalinolen buildable unknown x,x
 alphaglycerophosph|lalphaglycerophosph|dalphaglycerophosph|dlalphaglycerophosph
 buildable unknown x,x
 alphaglycerophospho|lalphaglycerophospho|dalphaglycerophospho|dlalphaglycerophos
 pho buildable unknown x,x
 betaoestradiol|betaestradiol buildable unknown x,x
 dicarboxylicimide|dicarboxylicacidimide buildable unknown x,x
 hydrogentartrate|hydrogenltartrate|hydrogendtartrate|lbitartrate|dbitartrate|hyd
 rogenmaleate|hydrogenoxalate|hydrogensulfate|hydrogensulfite|hydrogensulfide
 buildable unknown x,x
 alphaionon|alphaionone|betaionone|betaionon buildable unknown x,x
 sulfurdiimide|sulfurdiimid buildable unknown x,x
 snglycerol|snglycero|racglycerol|racglycero buildable unknown x,x
 orthophosphor buildable unknown x,x
 uvgrade buildable unknown x,x
 ionchromatography buildable unknown x,x
 dewarbenzene buildable unknown x,x
 alloisoleuc|allothreono|allothreon buildable unknown x,x
 anaphthoflavone|alphanaphthoflavone|bnaphthoflavone|betanaphthoflavone buildable
 unknown x,x
 gcstandard|primarystandard|secondarystandard buildable unknown x,x
 purineriboside buildable unknown x,x
 secpheneth buildable unknown x,x
 4nitroanilide|pnitroanilide buildable unknown x,x
 betacitronell buildable unknown x,x
 methylviologen|ethylviologen|benzylviologen buildable unknown x,x
 zirconyliv|vanadyliv buildable unknown x,x

activatedcarbon|onactivatedcarbon buildable unknown x,x
 extrapure buildable unknown x,x
 maycontain buildable unknown x,x
 volumetricstandard buildable unknown x,x
 notstabilized buildable unknown x,x
 zonerefined buildable unknown x,x
 standardsolution buildable unknown x,x
 wt buildable unknown x,x
 phosphorustriamide buildable unknown x,x
 nepsilon buildable unknown x,x
 betacarboline buildable unknown x,x
 pentamethylenetetramine|pentamethylenetetramin buildable unknown x,x
 hexamethylenetetramine|hexamethylenetetramin buildable unknown x,x
 ochloranil|mchloranil|pchloranil buildable unknown x,x
 mesoinositol|myoinositol|dinositol|linositol|scylloinositol|epiinositol
 buildable unknown x,x
 stainlesssteel buildable unknown x,x
 alphafuril buildable unknown x,x
 alphapinene|betapinene buildable unknown x,x
 chrysoidiner buildable unknown x,x
 naphtholas buildable unknown x,x
 neutralbuffer buildable unknown x,x
 alphacumyl buildable unknown x,x
 alphaphellandrene|betaphellandrene buildable unknown x,x
 bisphenola buildable unknown x,x
 alphalip|alip buildable unknown x,x
 alpharesorcyl|aresorcyl|betaresorcyl|bresorcyl|gammaaresorcyl|gresorcyl buildable
 unknown x,x
 gerani buildable unknown x,x
 lascorb buildable unknown x,x
 vitaminh|vitaminb1|thiaminedisulfide|vitaminb2|vitamine|alphatocopherol|atocophe
 rol buildable unknown x,x
 vitamind3 buildable unknown x,x
 phenolsulfonphthalein|phenolsulfonephthalein|m cresolsulfonphthalein|m cresolsulfo
 nephthalein|ocresolsulfonphthalein|ocresolsulfonephthalein|pyrocatecholsulfonpht
 halein|pyrocatecholsulfonephthalein|pyrogallolsulfonphthalein|pyrogallolsulfonep
 hthalein|thymolsulfonphthalein|thymolsulfonephthalein|phenolphthalein|m cresolpht
 halein|ocresolphthalein|pyrocatecholphtalein|pyrogallolphthalein|thymolphthalei
 n buildable unknown x,x
 freeradical buildable unknown x,x
 obenzeno buildable unknown x,x
 ptoluquinone|pxyloquinone buildable unknown x,x
 cyclopentaaphenanthrene|cyclopentaaphenanthren buildable unknown x,x
 pdioxine|mdioxine|pdioxin|mdioxin buildable unknown x,x
 asindacene|asindacen|sindacene|sindacen buildable unknown x,x
 sendachromeal buildable unknown x,x
 isonicotino|isonicotin buildable unknown x,x
 leucicacid buildable unknown x,x
 isoser buildable unknown x,x
 isoval buildable unknown x,x
 isoleuc buildable unknown x,x
 tleuc|tertleuc buildable unknown x,x
 orthotyros buildable unknown x,x
 mtyros|metatyros buildable unknown x,x
 ptyros|paratyros buildable unknown x,x
 hydroxyprol|3hydroxyprol|4hydroxyprol|5hydroxyprol buildable unknown x,x
 3phenylalan|betaphenylalan buildable unknown x,x

dtartar|dtartr|mesotartar|mesotartr buildable unknown x,x
 tetrafluoroborate|tetrafluoroborate1 buildable unknown x,x
 fluorosilicate|fluorosilicat|hexafluorosilicate|hexafluorosilicat buildable
 unknown x,x
 onnazoxy|nnoazoxy|nonazoxy buildable unknown x,x
 glycolacetal|glycolketal buildable unknown x,x
 moll|mgml|microgml|glt|reagentfor|reagentacs|acsreagent buildable unknown x,x
 ptosylate|ptosyl buildable unknown x,x
 oxazine1|oxazine4 buildable unknown x,x
 tboc buildable unknown x,x
 iumion|ideion|iumcation|ideanion buildable unknown x,x
 isobutyro|isobutyr buildable unknown x,x
 isovalero|isovaler buildable unknown x,x
 isophthalo|mpththalo|isophthal|mpththal buildable unknown x,x
 terephthalo|pphthalo|terephthal|pphthal buildable unknown x,x
 etherof buildable unknown x,x
 esterswith|estersof|esterwith|esterof buildable unknown x,x
 saltof buildable unknown x,x
 iclactone|iclacton buildable unknown x,x
 iclactam buildable unknown x,x
 anhydridewith buildable unknown x,x
 cyclicanhydride buildable unknown x,x
 phosphoruspentoxide buildable unknown x,x
 allcis buildable unknown x,x
 alltrans buildable unknown x,x
 acinitro buildable unknown x,x
 astriazine|astriazin|striazine|striazin|asymtriazine|asymtriazin|symtriazine|sym
 triazin buildable unknown x,x
 astrioxane|astrioxan|strioxane|strioxan|asymtrioxane|asymtrioxan|symtrioxane|sym
 trioxan buildable unknown x,x
 astriazino|striazino|asymtriazino|symtriazino buildable unknown x,x
 astrioxano|strioxano|asymtrioxano|symtrioxano buildable unknown x,x
 astrithiane|astrithian|strithiane|strithian|asymtrithiane|asymtrithian|symtrithi
 ane|symtrithian buildable unknown x,x
 thiurammonosulfide|thiuramdisulfide|thiuramtrisulfide|thiuramtrisulfid|thiuramte
 trasulfide|thiuramtetrasulfid buildable unknown x,x
 isourea|isothiourea|lisoureido|3isoureido|1isothioureido|3isothioureido|1isosele
 noureido|3isoselenoureido|1isotelluroureido|3isotelluroureido buildable unknown
 x,x
 ' typo typo '
 " typo typo ''
 ± typo typo +/-
 μ typo typo mu
 , - typo typo -
 § typo typo beta
 -> typo typo -fwdarw-
 (alpha) typo typo alpha
 (beta) typo typo beta
 (gamma) typo typo gamma
 (delta) typo typo delta
 (epsilon) typo typo epsilon
 (omega) typo typo omega
 (ortho) typo typo ortho
 (meta) typo typo meta
 (para) typo typo para
 (tau) typo typo tau
 -oxyl typo typo -oxylradical

[illegible]

[illegible]

threonic typo typo threonic
 tricaprin typo typo tricapr-in
 tricaproin typo typo trihexanoin
 trichloromethylsulfen|trichloromethanesulfen typo typo (trichloromethyl)sulfen
 trifluoromethylsulfen|trifluoromethanesulfen typo typo (trifluoromethyl)sulfen
 trioleate typo typo (tris)oleate
 triolein typo typo tri-ole-in
 trioleoyl typo typo (tris)oleoyl
 trioleyl typo typo (tris)oleyl
 triphosphate typo typo triphosphate
 trithioperoxy typo typo thiodithioperoxy
 tritolyl typo typo tristolyl
 tropilidene typo typo 2,4,6-cyclohexatriene
 tyrosinate typo typo tyrosin-ate
 uloson typo typo ulo-on
 xanthylic typo typo xanthonylic
 xylul typo typo threopentul
 acidic notthisversion unknown x,x
 activatedcarbon notthisversion bulksolid x,x
 agarose notthisversion macromolecule x,x
 agar notthisversion macromolecule x,x
 agglutinin notthisversion macromolecule x,x
 albumin notthisversion macromolecule x,x
 alkonium notthisversion mixture x,x
 alkyl|alkyl* notthisversion mixture x,x
 alloy notthisversion bulksolid x,x
 algin notthisversion macromolecule x,x
 alumina notthisversion bulksolid x,x
 amalgam notthisversion bulksolid x,x
 amyloid notthisversion macromolecule x,x
 amylose notthisversion macromolecule x,x
 angiotensin notthisversion macromolecule x,x
 anthocyanidin notthisversion mixture x,x
 anthocyanin notthisversion mixture x,x
 antibody notthisversion macromolecule x,x
 antibovine notthisversion macromolecule x,x
 anticat notthisversion macromolecule x,x
 antichickens notthisversion macromolecule x,x
 antidog notthisversion macromolecule x,x
 antigoat notthisversion macromolecule x,x
 antiguineapig notthisversion macromolecule x,x
 antihorse notthisversion macromolecule x,x
 antihuman notthisversion macromolecule x,x
 antimonkey notthisversion macromolecule x,x
 antirabbit notthisversion macromolecule x,x
 antirat notthisversion macromolecule x,x
 antisheep notthisversion macromolecule x,x
 ase notthisversion macromolecule x,x
 asphalt notthisversion mixture x,x
 avidin notthisversion macromolecule x,x
 azure notthisversion color x,x
 bacitracin notthisversion macromolecule x,x
 bead|beads notthisversion bulksolid x,x
 bentonite notthisversion bulksolid x,x
 black notthisversion color x,x
 block notthisversion polymer x,x
 blue notthisversion color x,x

bombesin notthisversion macromolecule x,x
 bradykinin notthisversion macromolecule x,x
 brij notthisversion polymer x,x
 brilliant notthisversion color x,x
 bromelian notthisversion macromolecule x,x
 broth notthisversion mixture x,x
 brown notthisversion color x,x
 buckyball|buckyballs notthisversion fullerene x,x
 buffer notthisversion mixture x,x
 calcia notthisversion bulksolid x,x
 calcitonin notthisversion macromolecule x,x
 carborundum notthisversion bulksolid x,x
 carmine notthisversion color x,x
 carrageenan notthisversion macromolecule x,x
 casein notthisversion macromolecule x,x
 casomorphin notthisversion macromolecule x,x
 celite notthisversion bulksolid x,x
 cells notthisversion bulksolid x,x
 cellulose notthisversion macromolecule x,x
 cephalin|cephalins notthisversion mixture x,x
 ceria notthisversion bulksolid x,x
 charcoal notthisversion bulksolid x,x
 chelate notthisversion mixture x,x
 chitin notthisversion macromolecule x,x
 chitosan notthisversion macromolecule x,x
 cholecystokinin notthisversion macromolecule x,x
 chondroitin notthisversion macromolecule x,x
 cocktail notthisversion mixture x,x
 coco notthisversion mixture x,x
 collagen notthisversion macromolecule x,x
 collodion notthisversion macromolecule x,x
 concanavalin notthisversion macromolecule x,x
 conotoxin notthisversion macromolecule x,x
 demi notthisversion hemi x,x
 detergent|detergent notthisversion mixture x,x
 dextrin|dextran notthisversion macromolecule x,x
 dna notthisversion macromolecule x,x
 dowex notthisversion polymer x,x
 drierite notthisversion bulksolid x,x
 dynorphin notthisversion macromolecule x,x
 edestin notthisversion macromolecule x,x
 endorphin notthisversion macromolecule x,x
 endothelin notthisversion macromolecule x,x
 enzyme|enzymes notthisversion macromolecule x,x
 emulsin notthisversion macromolecule x,x
 extract notthisversion mixture x,x
 fatty notthisversion mixture x,x
 ferritin notthisversion macromolecule x,x
 fibrin notthisversion macromolecule x,x
 fibrinogen notthisversion macromolecule x,x
 fibrinolysin notthisversion macromolecule x,x
 fibronectin notthisversion macromolecule x,x
 ficin notthisversion macromolecule x,x
 ferrocene|ferrocen notthisversion inorgcomplex x,x
 flavor notthisversion mixture x,x
 fraction notthisversion mixture x,x
 fullerene|fullerenes notthisversion fullerene x,x

vasopressin notthisversion macromolecule x,x
venom notthisversion mixture x,x
violet notthisversion color x,x
wax notthisversion bulksolid x,x
white notthisversion color x,x
xylan notthisversion macromolecule x,x
yeast notthisversion bulksolid x,x
yellow notthisversion color x,x
yttria notthisversion bulksolid x,x
zein notthisversion macromolecule x,x
zeolite notthisversion bulksolid x,x
zephiran notthisversion macromolecule x,x
zephirol notthisversion macromolecule x,x
zirconia notthisversion bulksolid x,x
zyme notthisversion macromolecule x,x
ortho ordinal ordinal x,x
epsilon ordinal ordinal x,x
nepi ordinal ordinal x,x
npi ordinal ordinal x,x